

MAGNETO-OPTICAL STUDIES IN  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$   
SEMICONDUCTING ALLOYS

BY

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in Physics.

ABSTRACT

Interband magneto-optical absorption in the Voigt and the Faraday configuration has been studied near liquid-helium temperature in samples of  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  grown by liquid-phase epitaxy on InP substrates and are reported here in two samples with  $(x=0.25, y=0.52)$  and  $(x=0.47, y=1)$ . The magnetotransmission spectra were analyzed using the quasi-Ge model with exciton corrections. It is found that such measurements determine  $E_g$ ,  $1/\mu_+ \equiv (1/m_c + 1/m_{\ell h})$ , and  $1/\mu_- \equiv (1/m_c + 1/m_{hh})$ , and therefore  $m_c$  and  $m_{\ell h}$ , within a narrow range ( $m_{hh} \gg m_c$  and  $m_{\ell h}$ ). The anisotropy factor  $\gamma_3 - \gamma_2$  is also determined within a narrow range when measurements are performed with H oriented along two different crystal axes. Using a minimization routine the following quasi-Ge parameters were obtained. For  $(x=0.25, y=0.52)$ :  $E_g = 1065 \pm 1$  meV,  $m/\mu_- = 18.8 \pm 0.5$ ,  $m/\mu_+ = 29.5 \pm 0.5$ . Assuming  $(m_{hh}/m)_{100} = 0.45 \pm 0.05$ ,  $\Delta = 0.24 \pm 0.01$  eV, and  $E_p$  between 17.5 and 25.8 eV ( $F=0$  to  $-3.5$ ) we obtain  $m_c/m = 0.0602 \pm 0.001$ ,  $m_{\ell h}/m = 0.078 \pm 0.001$ ,  $g_c = -0.06$  to  $-1.25$ .  $\gamma_3 - \gamma_2 = 0.35$  or  $0.7$  gave the same values, within the error bars, for the above parameters. (Only  $\vec{H} \parallel [100]$  data were taken). With  $\gamma_3 - \gamma_2 = 0.7$ ,  $\gamma_1^L = 7.5 \pm 0.3$ ,  $\gamma_2^L = 2.4 \pm 0.1$ ,  $\gamma_3^L = 3.1 \pm 0.1$ ,  $\kappa^L = 1.5 \pm 0.1$ . For  $(x=0.47, y=1)$ :  $E_g = 813 \pm 1$  meV,  $m/\mu_- = 26.1 \pm 0.5$ ,  $m/\mu_+ = 43.4 \pm 1.0$ .  $\gamma_3 - \gamma_2 = 0.8 \pm 0.2$ . With  $(m_{hh}/m)_{100} = 0.45 \pm 0.05$ ,  $\Delta = 0.35 \pm 0.01$  eV, and  $E_p$  between 21 and 27 eV ( $F=0$  to  $-3.5$ ) we obtained  $m_c/m = 0.0415 \pm 0.0015$ ,  $m_{\ell h}/m = 0.0515 \pm 0.0015$ ,  $g_c = -3$  to  $-5$ ,  $\gamma_3 - \gamma_2 = 0.8 \pm 0.05$ ,  $\gamma_1^L = 10.6 \pm 0.2$ ,  $\gamma_2^L = 4.0 \pm 0.1$ ,  $\gamma_3^L = 4.8 \pm 0.1$ ,  $\kappa^L = 3.3 \pm 0.1$ .

$E_p$  could not be precisely determined even when the nonparabolicity of the conduction band was examined. A precise measurement of  $E_p$  requires precise measurements of  $g_c$ .

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*To My Parents*

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CHAPTER IINTRODUCTION

In this thesis we report on the interband magnetoabsorption measurements carried out in two members of the family of semiconducting III-V alloys  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  which are grown by liquid phase epitaxy lattice matched to InP substrates.

One of the motivating factors for this investigation is that the  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  quaternary alloys have recently become technologically important semiconductor materials for optoelectronic devices because of (1) wide variation of the bandgap between 0.36 and 2.2 eV by varying the composition parameters  $x$  and  $y$ , and (2) lattice-matched epitaxial growth on GaAs or InP substrates. These materials have been used successfully for the fabrication of a number of important devices such as light emitting diodes,<sup>1,2</sup> photocathodes,<sup>3</sup> photodiodes,<sup>4</sup> Gunn oscillators,<sup>5</sup> and double heterojunction lasers.<sup>6,7</sup>

An important application of the  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  quaternary epitaxial films is in the field of fiber-optics communications, since using these materials it is possible to fabricate lasers and detectors which operate in the wavelength region corresponding to the region of minimum loss and minimum dispersion of optical fibers. Until recently, this has been the 1.2  $\mu\text{m}$  region,<sup>8,9</sup> corresponding to 1.0 eV. More recently, however, fibers have been developed whose optimal operation region lies in the longer wavelength region

corresponding to alloy compositions closer to the  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  end of the family.<sup>10</sup>

Another aspect of these quaternary materials which is interesting from the point of view of device application as well as physics of III-V semiconductors is the fact that in addition to the band gap, other electronic band parameters for these materials can be varied by varying the alloy composition.

A potentially interesting application of these materials from both device and physics point of view is to the fabrication of super-lattices. The evidence for the growth of interest in these materials comes from the increase in the number of contributions in the literature in recent years dealing with this alloy family.<sup>11</sup> The first systematic measurements of the relationship between  $x$  and  $y$  and the laser emission photon energies at temperatures of 300K and 80 K for the quaternaries lattice matched to InP were obtained by Hsieh.<sup>12</sup> Nahory et al<sup>13</sup> used photoluminescence spectra to measure energy gaps, as well as the lattice matching condition. The lattice matching condition is generally taken to be  $y \approx 2.2x$  or  $x \approx 0.47y$ .

The first measurement of the effective mass in a member of this alloy family was reported by Restorff et al<sup>14</sup> who deduced a value of  $m_c = 0.060 m$  (where  $m$  is the free electron mass) from the temperature dependence of the amplitude of weakly resolved Shubnikov-de Haas measurements in a quaternary sample with composition parameters  $x=0.10$ ,  $y=0.22$ .

At very nearly the same time that we reported our first interband magnetoabsorption measurements of these materials ( $x=0.25$ ,  $y=0.52$ ),<sup>15</sup> Portal et al<sup>16</sup> reported measurements of the effective masses of four members of the alloy family using magnetophonon resonance, Shubnikov-de Haas oscillations, and cyclotron resonance. Our effective mass value of  $m_c=0.061 m$  and those of Ref. 16. suggested very strongly a linear variation of  $m_c$  with  $y$  for  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  alloys lattice matched to InP. In fact, Nicholas et al<sup>17</sup> suggested the empirical relationship  $m_c(y)=(0.080 - 0.039y) m$ . It was noted<sup>16,17</sup> that the value of  $m_c$  for samples with  $x=0.12$  and  $y=0.23$  reported in Ref. 16 was 0.072, 20% higher than the value reported earlier in Ref. 14 for  $x=0.10$ ,  $y=0.22$ . Furthermore, the value of  $m_c=0.038 m$  estimated by Nishino et al<sup>18</sup> from electro-reflectance studies of an alloy with  $x=0.21$ ,  $y=0.54$  fell well below our value of 0.061m for  $x=0.25$ ,  $y=0.52$ . In a more recent publication by Brendecke et al<sup>19</sup> cyclotron resonance results were reported and effective masses were deduced giving values between 20% and 30% below the linear interpolation. Shubnikov-de Haas measurements reported by Perea et al<sup>20</sup> were closer to the linear interpolation with a small downward bowing which was about 9% at the most. The more recent Shubnikov-de Haas measurements of Restorff et al<sup>21</sup> were also in better agreement with the linear interpolation compared to the previously reported results of Ref. 14. In a very recent article, Nicholas et al<sup>22</sup> have reported cyclotron resonance and magnetophonon resonance measurements of the effective mass  $m_c$  for several members of the alloy family over the whole range  $y=0.23$  to  $y=1$  for lattice matched samples. These results agree very well with

the linear interpolation for  $m_c$  mentioned above and as pointed out in Ref.22, our result<sup>15</sup> is in agreement with theirs. Furthermore, in Ref. 22, the authors show evidence that the low masses deduced by Ref. 19 result from an observation of an impurity transition which is dominant for lattice temperatures below 30K. In summary, our results and those of Refs. 16, 17 and 22, are in excellent agreement with the linear interpolation for  $m_c$ .

Interband magneto-optics has played an important role in providing a quantitative understanding of important energy bands in semiconductors. The interband magneto-optical effects have been the subject of extensive experimental and theoretical investigations. Extensive references to these important contributions can be found in the review articles by Lax and Mavroides,<sup>23</sup> and Aggarwal.<sup>24</sup> One feature of magneto-optics is the richness of the spectra as a result of optical transitions between the  $a^\pm(n')$ ,  $b^\pm(n')$ ,  $a^{SO}(n')$ , and  $b^{SO}(n')$  series of the heavy (-), light (+), and the spin-orbit split-off (so) valence band magnetic sublevels to the conduction band  $a^C(n)$  and  $b^C(n)$  magnetic sublevels. This enables one to extract a lot of information about these bands by examining interband magneto-optical spectra as a function of light polarization and crystal axis orientation with respect to the magnetic field, provided the samples are of high enough quality to allow some of these features to be resolved. Therefore, one aspect of our initial objective was to determine whether these alloy semiconductors can indeed be amenable to magneto-optical studies and whether they could provide

magneto-optical spectra with enough structure to enable us to obtain some of the band parameters. This thesis reports on such studies and indicates that there is a great potential for applying the rich method of interband magneto-optics to this alloy family. We bring to attention the results for one of our quaternary samples<sup>15</sup> and those for a ternary  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  sample,<sup>25,26</sup> which are described in this thesis. We have also obtained room temperature electro-reflectance spectra for a number of quaternary samples using the electrolyte method of Cardona et al<sup>27</sup> which we present in Appendix A. The signal to noise ratio and the presence of the onset of Franz-Keldysh oscillations<sup>28</sup> point to the high quality of samples available to us (for example compare spectra in Appendix A with those reported in the literature). These studies of electroreflectance, although preliminary, are encouraging and suggest that magneto-electroreflectance measurements<sup>29,30</sup> for both the fundamental edge and the split-off edge would be possible in these alloys. Stress modulated magnetoreflexion measurements may also turn out to be possible.<sup>31</sup>

Interband magneto-optical measurements, as mentioned before, have been extensively used to determine band parameters of semiconductors. The model which is most applicable for the analysis of these spectra is the "Quasi-Ge" coupled band model of Pidgeon and Brown,<sup>32</sup> with the improvements incorporated by Weiler.<sup>33</sup> The band parameters we shall refer to are those which appear in Ref.33 for example. In Chapter II of this thesis a review of the "quasi-Ge"

model, based on Ref. 33, will be given. In Chapter III, we present our magnetoabsorption experiments in two members of the alloy family. In Chapter IV, we present analysis of our magnetoabsorption experiments based on the quasi-Ge model. The presentation in this thesis would be similar to those in Refs. 31 and 33. In addition, we include a discussion of the effect of higher bands on our measurements. In Chapter V, we give a summary of the results and suggestions for future work. In Appendix A, electroreflectance spectra for a few quaternary samples will be presented. The remaining Appendices, will be dealing with some of the details of Chapter IV and the nonparabolicity of the conduction band.

Briefly, the band parameters which are readily obtained (within a few per cent or less) from interband magneto-optical measurements (in the absence of well resolved spectra from the spin-orbit split-off band to the conduction band transitions) are the following: the energy gap  $E_g$ , the reduced effective masses  $(1/\mu_{\pm})=(1/m_c)+(1/m_{\pm})$  for the conduction and heavy (-) or light (+) hole bands, and the anisotropy factor  $\gamma_3-\gamma_2$ . Since  $m_-$  is quite large compared to  $m_c$  (by a factor of  $\sim 10$ )  $1/\mu_-$  determines  $m_c$  within a narrow range, thus the value of  $m_+$  is also determined within a narrow range.

Another important parameter is  $E_p$ , the interband transition energy, which is proportional to the square of momentum matrix element between valence and conduction bands. Since the effect of

higher bands is quite small on  $g_c$ , the conduction band  $g$ -factor,<sup>33,34</sup> the measured value of  $g_c$  can be used to obtain  $E_p$  provided the  $g$ -factor values are measured to a good degree of precision and the spin-orbit splitting energy  $\Delta$  and the energy gap  $E_g$  measurements are available. On the other hand, since the effect of high bands on the curvature (effective mass) of the conduction band could be as large as 20% of that due to the valence bands,  $m_c$  cannot precisely determine  $E_p$ . However, magneto-optical measurements can determine  $E_p$  to within about 20%. We have found that a linear interpolation of the values of  $E_p$  from the binaries InAs, GaAs, and InP can give good fits to our data. Ignoring the effect of higher bands, which would predict a smaller  $E_p$ , can also give good fits.

Recently, Hermann et al<sup>35,36</sup> have applied the technique of optical pumping for the measurements of valence band spin-orbit splitting in several samples of  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  over the range  $y=0$  to 1 and their values for  $m_c$ ,  $m_+$  (lighthole effective mass), and

$$\bar{\beta} \equiv \frac{1}{3} \frac{(3/\mu_+) + (1/\mu_-)}{(1/\mu_+) - (1/\mu_-)}$$

are in excellent agreement with the values we have obtained for our quaternary and ternary samples. For  $g_c$  a preliminary value of  $(-4.2 \pm 25\%)$  has been obtained<sup>36</sup> for the ternary  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ , again in very good agreement based on interpolated value of  $E_g$  which we had used for the ternary, however, work is being done to reduce the error-bars on  $g_c$ .<sup>36</sup>

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CHAPTER IITHEORETICAL BACKGROUNDA. Introduction

The effect of a magnetic field on the energy bands of a semiconductor particularly as it affects the interaction of electromagnetic radiation with these materials has been the subject of a great deal of theoretical and experimental studies. The impetus for the vast amount of research in this area was the early intraband cyclotron resonance experiment first carried out at microwave frequencies,<sup>1,2</sup> and later at infrared wavelengths.<sup>3,4</sup> In this thesis we are interested in optical transitions (in the infrared region) from the valence bands' magnetic sublevels to the conduction band's magnetic sublevels, corresponding to the fundamental gap of a semiconductor in the presence of an external magnetic field. This is in general referred to as interband magneto-optics. The interband magneto-optical effects have been the subject of extensive experimental and theoretical investigations. Extensive references to these important contributions can be found in the review articles by Lax and Mavroides<sup>5</sup> and Aggarwal.<sup>6</sup>

Specifically, we are interested in a theory which enables us to calculate the energies of the above mentioned magnetic sublevels for a direct gap III-V semiconductor of the zinc-blende type (point group symmetry  $T_d$ ) with the fundamental gap occurring

at the Brillouin zone center ( $\vec{k}=0$ )

The theory we shall use to interpret our magnetoabsorption experiments is the coupled-band quasi-Ge model based on the  $\vec{k}\cdot\vec{p}$  perturbation theory carried out by Pidgeon and Brown<sup>7</sup> and later modified by Weiler<sup>8</sup> and coworkers.<sup>9</sup>

In Section B we give a brief review of  $\vec{k}\cdot\vec{p}$  theory for zinc-blende semiconductors leading to the quasi-Ge model Hamiltonian of P.B. modified by Weiler. In Section C we give some of the results of the quasi-Ge model. In Section D the selection rules for optical transitions will be given.

#### B. Effective-Mass Theory and the Magnetic Field -- $\vec{k}\cdot\vec{p}$ Theory For Zinc-Blende Semiconductors

A principal approach to describing the motion of charged carriers in a perturbed periodic potential is the effective-mass theory. In this method, the effect of the periodic potential on the dynamics of the charged carrier is replaced by terms which appear in the equation of motion much in the same way that mass appears in the case of free electron. In the simplest case these constants take the form of a mass tensor. In the case of degenerate or nearly degenerate bands, the effective-mass constants appear in a more complicated form. In the effective-mass method of Luttinger and Kohn (L.K.)<sup>10</sup> the motion of an electron in a perturbed periodic potential (e.g., electron in a semiconductor in the presence of an external magnetic field) was considered

and effective-mass Hamiltonian was obtained, including the  $\vec{k} \cdot \vec{p}$  and spin-orbit terms.

### B. 1. A Brief Review

Before we give the formalism of the coupled band quasi-Ge model we review some of the work which led to that of P.B. and Weiler for the case of zinc-blende type semiconductors. In the case of InSb, with band extrema at the fundamental gap at the Brillouin zone center, in the absence of an external magnetic field, Kane<sup>11</sup> did the following. He considered the Schrödinger equations for the cell periodic functions, including the  $\vec{k} \cdot \vec{p}$  and the spin-orbit interaction terms. For  $\vec{k}=0$  he used the single-group basis functions of the  $T_d$  group. He explicitly considered basis states  $\Gamma_1$  (S for conduction band) and  $\Gamma_4$  (X,Y,Z for valence bands) for  $\vec{k}=0$  at the fundamental edge. Including up and down spin wave functions he obtained two degenerate sets of four basis functions and for the  $\vec{k} \cdot \vec{p}$  Hamiltonian obtained two 4x4 matrices. In these matrices he considered all possible matrix elements of the  $\vec{k} \cdot \vec{p}$  as well as the spin-orbit term between these  $\Gamma_1$  and  $\Gamma_4$  functions (S,X,Y,Z) of the fundamental edge up to second order in  $\vec{k}$ . The first-order matrix elements coupled different members of the (S,X,Y,Z) set. The second-order terms included not only these four functions, but also the higher bands as intermediate states. For the case of these higher bands spin-orbit splitting was ignored and single-group basis functions  $\Gamma_1'$ ,

$\Gamma_3'$ ,  $\Gamma_4'$ , and  $\Gamma_5'$  appeared in Kane's treatment (prime indicates higher bands). The effect of these higher bands appeared as band parameters in the 4x4 Hamiltonians of Kane and the effect of spin-orbit splitting was included only in the conduction and valence bands of the fundamental gap. The effect of higher bands appeared only as coefficients multiplying  $k^2$  terms in the 4x4 Hamiltonian matrices. (For Kane band parameters see Appendix B.) The Hamiltonian was then expressed in terms of linear combinations of X, Y, Z and the spin-functions  $\uparrow$  and  $\downarrow$ , which diagonalized the spin-orbit interaction.

A second approach was chosen by Luttinger,<sup>12</sup> who used group theory with the double-group representation of  $T_d$  to obtain all of the allowed matrix elements of  $\vec{k}$  and  $\vec{k}x\vec{k}$  among the four-fold degenerate valence band states transforming as the  $\Gamma_8$  double-group representation of  $T_d$ . The intermediate states (which included the  $\Gamma_6$  conduction band) were also taken in the double-group representation. His results involved band parameters which were linear combinations of those of Kane, but in addition included a parameter  $q$ , which is nonzero only in the presence of spin-orbit splitting of the intermediate states. Since he considered coupling only among  $\Gamma_8$  valence band state, Luttinger obtained a 4x4 matrix. Roth, Lax, and Zwerdling (R.L.Z.)<sup>13</sup> improved the treatment by including also the spin orbit split-off band  $\Gamma_7$ , but still leaving the  $\Gamma_6$  conduction band as an intermediate state

(getting a 6x6 Hamiltonian). Pidgeon and Brown<sup>7</sup> included the  $\Gamma_6$  conduction band in their analysis (8x8 Hamiltonian). However, they ignored the spin-orbit splitting of the intermediate states. Thus, P.B. combined Kane's method of calculating bands for  $H=0$  with R.L.Z.'s method of treating the magnetic field in the coupled-band scheme. Thus, P.B. included the coupling between the conduction and valence bands exactly, and the effect of higher bands to order  $k^2$ . In this manner the effects of nonparabolic conduction and light-hole bands, warping of the conduction and valence bands, and the quantum effects of light- and heavy-hole valence bands were included. Their 8x8 Hamiltonian does not include  $q$  and higher term corrections to the conduction band  $g$ -factor, i.e.,  $N_1$ . The 8x8 Hamiltonian can, under certain approximation, be broken into two 4x4 block diagonal Hamiltonians; the so-called quasi-Ge model Hamiltonians.

In Weiler's<sup>8,9</sup> treatment (unlike in P.B.) the spin-orbit interaction as regards to its effect on the symmetries of the intermediate states was not ignored. In this treatment, the double-group basis states  $\Gamma_6$  (for the conduction band),  $\Gamma_8$  (for the heavy and light hole valence bands) and  $\Gamma_7$  (for the spin-orbit split-off valence band) were used, both for the fundamental edge bands and the intermediate bands. Thus an 8x8 matrix was obtained with  $\Gamma_6^C$ ,  $\Gamma_8^V$ , and  $\Gamma_7^V$  as its basis ( $c$  refers to conduction band and  $v$  to valence band, see Figure II-1). These basis

functions are given in Table II-1.

To obtain the 8x8 Hamiltonian group theoretical analysis was used utilizing tables of Koster, Dimmock, Wheeler, and Statz, (K.D.W.S.)<sup>14</sup> to find all of the allowed matrix elements of  $\vec{k}$  and  $\vec{k} \times \vec{k}$  among the  $\Gamma_6$ ,  $\Gamma_7$ , and  $\Gamma_8$  basis states of the double-group representation of  $T_d$  and a complete set of independent parameters were obtained (see Table II-2). These include, in addition to the P.B. parameters and  $q$ , three additional small parameters  $N_1$ ,  $N_2$ , and  $N_3$  where  $N_1$  is the contribution of the higher bands to the conduction band  $g$ -factor  $g_c$  and is nonzero only in the presence of spin-orbit splitting of the higher bands, and  $N_2$  and  $N_3$  are two inversion assymetry parameters. In the rest of Section B we give a brief account of the formalism of the  $\vec{k} \cdot \vec{p}$  theory in a zinc-blende type semiconductor (point group symmetry  $T_d$ ) in the vicinity of the zone center ( $\vec{k}=0$ ) near the fundamental gap, in the presence of an external magnetic field  $H$ , up to second order in  $k$  and first order in  $H$ , as presented in Weiler's thesis. We also compare the two 4x4 quasi-Ge Hamiltonians for the a- and b- sets obtained from the 8x8 Hamiltonian under certain approximations with those given by P.B. who neglect terms involving  $N_1$  and  $q$ . For the purpose of analyzing our experiments we have used Weiler's quasi-Ge model Hamiltonians which include  $N_1$  and  $q$ , although it turns out that for the physically reasonable range of  $N_1$  and  $q$ , our experimental data

are insensitive to these two parameters. This will be discussed further in Chapter IV and Appendix B.

### B. 2. The Effective-Mass Hamiltonian

The envelope functions  $f_j(\mathbf{r})$  are the solutions of the effective-mass Hamiltonian. This is given below up to second-order in  $k$  and first-order in  $H$ , according to the L.K.<sup>10</sup> method as given in P.B.<sup>7</sup>

$$\sum_{j'} \left\{ \hbar^2 D_{jj'}^{\alpha\beta} k_\alpha k_\beta + \frac{\hbar}{m} \pi_{jj'}^\alpha k_\alpha + \mu_B (\vec{H} \cdot \vec{\sigma})_{jj'} + \frac{\hbar}{4m^2 c^2} [(\vec{\sigma} \times \vec{\nabla} V) \cdot \vec{p}]_{jj'} + E_{j'} \delta_{jj'} \right\} f_{j'}(\vec{r}) = E_j f_j(\vec{r}) \quad (2-1)$$

where

$$D_{jj'}^{\alpha\beta} \equiv \frac{1}{2m} \delta_{jj'} + \frac{1}{m^2} \sum_{i \neq j, j'} \frac{\pi_{ji}^\alpha \pi_{ij'}^\beta}{E_{j'} - E_i} \quad (2-2)$$

and

$$\pi_{\ell\ell'} \equiv \int_{\text{unit cell}} u_{\ell 0}^*(\vec{r}) \left[ \vec{p} - \frac{\hbar}{4mc^2} (\vec{\nabla} V \times \vec{\sigma}) \right] u_{\ell' 0}(\vec{r}) d^3 r \quad (2-3)$$

The functions  $f_j(\vec{r})$  are envelope functions and the total zeroth order wave function is

$$\Psi(\vec{r}) = \sum_j f_j(\vec{r}) u_{j0}(\vec{r}) \quad (2-4)$$

The functions  $u_{j_0}(\vec{r})$  are the Bloch functions at  $\vec{k}=0$  and include both space and spin variables. The symbols used above are:

- $\alpha, \beta$  = x,y,z are the indices in a right-handed coordinate system (x,y,z) along the principal cubic axes.
- $\vec{r}$   $\equiv (r_x, r_y, r_z)$  is the position vector in the (x,y,z) system.
- $\vec{H}$   $\equiv$  The external static magnetic field  $= \vec{\nabla} \times \vec{A}$ .
- $\vec{A}$   $\equiv$  The vector potential, will be taken in the Landau gage.
- $\vec{\sigma}$   $\equiv$  Pauli spin matrices, e.g.,  $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ .
- $\mu_B$   $\equiv \frac{e\hbar}{2mc}$  = Bohr magneton.
- m  $\equiv$  Free electron mass.
- e  $\equiv$  Absolute value of electron charge.
- c  $\equiv$  Speed of light in vacuum.
- $\hbar$   $\equiv h/2\pi$ , where h is Planck's constant.
- V  $\equiv V(\vec{r})$  is the periodic crystal potential.
- $\vec{p}$   $\equiv -i\hbar\vec{\nabla} \equiv -i\hbar(\frac{\partial}{\partial r_x}, \frac{\partial}{\partial r_y}, \frac{\partial}{\partial r_z})$  is the momentum matrix element.
- $\vec{\pi}_{\ell\ell'}$   $\equiv$  Modified momentum matrix element between bands  $\ell$  and  $\ell'$  at  $\vec{k}=0$ , including spin-orbit interaction.
- $u_{\ell_0}(\vec{r})$   $\equiv$  The Bloch function at  $\vec{k}=0$  for the  $\ell$ 'th band. It has the periodicity of  $V(\vec{r})$ . These functions include the electron spin variable as well.

$j$  and  $j'$   $\equiv$  Indices which run over the two conduction bands ( $\Gamma_6^C$ ) the four valence bands ( $\Gamma_8^V$ ) and the two split-off bands ( $\Gamma_7^V$ ) of the fundamental gap.

$E_j$   $\equiv$  The energy of state  $j$  at  $\vec{k}=0$ .

$i$   $\equiv$  The index which runs over all higher bands, clearly  $i \neq j, j'$ .

$E_i$   $\equiv$  The energy of the  $i$ th state at  $\vec{k}=0$ , including spin-orbit interaction.

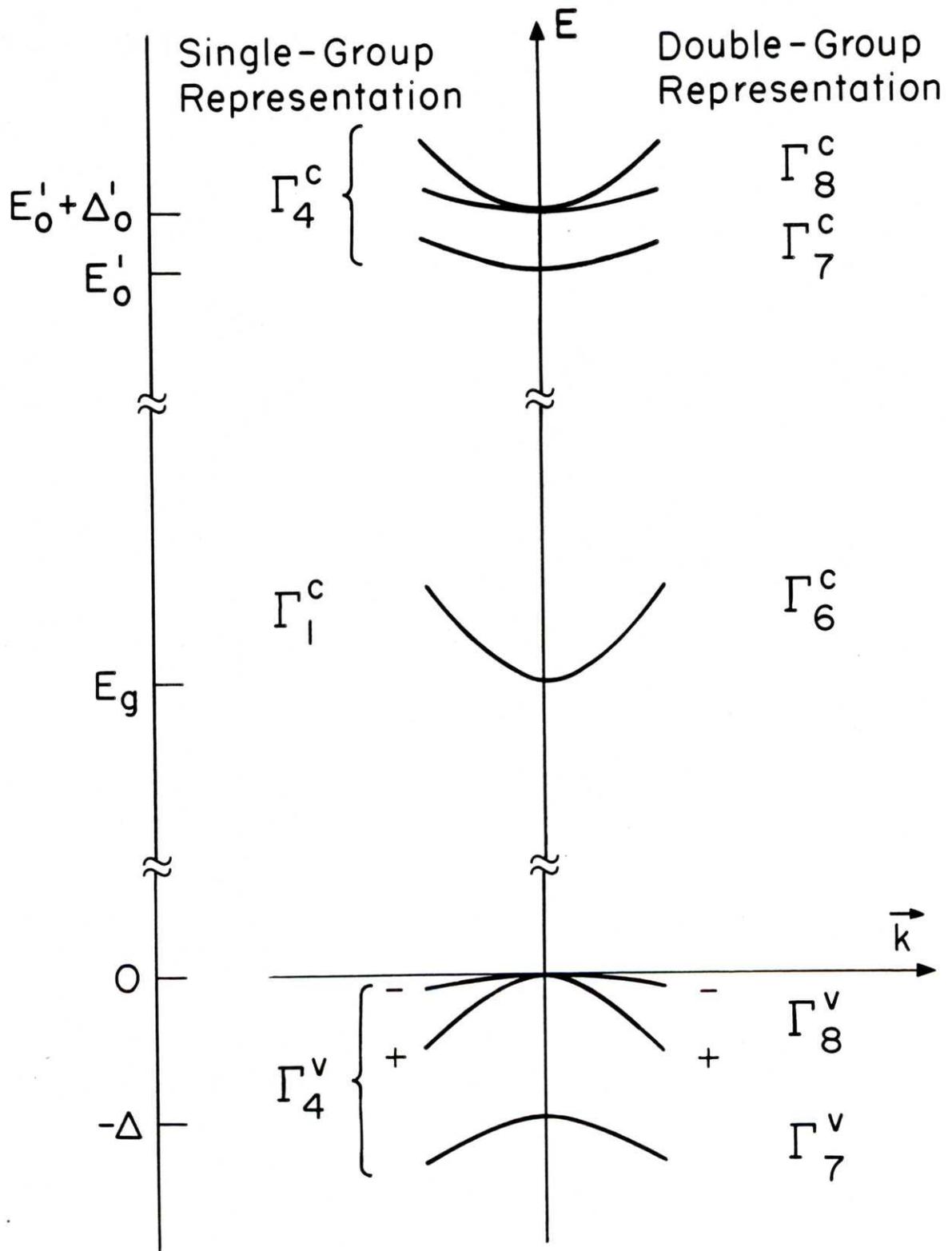
The terms involving subscript  $jj'$  are understood to be matrix elements between  $u_{j0}(\vec{r})$  and  $u_{j'0}(\vec{r})$ . Equation (2-1) is actually a set of eight equations since  $j$  refers to eight different bands. The sum over  $j'$  in Eq.(2-1) extends over the eight bands represented by  $j$  and  $j'$ . In the presence of a magnetic field, the operators  $\vec{K}(k_\alpha; \alpha=x,y,z)$  which appear in Eq.(2-1) are defined as

$$\vec{K} \equiv \frac{1}{\hbar} [\vec{p} + \left(\frac{e}{c}\right) \vec{A}] \quad (2-5)$$

Equation (2-2) defines the effective-mass tensor, the summation here is over  $i$ , all the intermediated (so-called higher) bands outside of the eight bands  $\Gamma_6^C$ ,  $\Gamma_8^V$ , and  $\Gamma_7^V$ , corresponding to the fundamental gap. The energy  $E_j$ , in the denominator is usually replaced by an average energy  $E_0$ . Equation (2-3) defines the modified momentum matrix element  $\vec{\pi}_{\ell\ell'}$ . The  $\Gamma_6$ ,  $\Gamma_7$ , and  $\Gamma_8$  are double-group representations of  $T_d$ .

FIGURE II-1 Schematic diagram of the band structure near  $\vec{k}=0$  in a direct gap zinc-blende type semiconductor at the fundamental gap  $E_g$ , at zero magnetic field. The bands which are explicitly treated by the  $8 \times 8$   $\vec{k} \cdot \vec{p}$  Hamiltonian are  $\Gamma_6^C$  conduction band (2-fold spin degenerate) the  $\Gamma_6^C$  valence band (4-fold degenerate at  $\vec{k}=0$ ) and the  $\Gamma_7^V$  split-off band (2 fold spin degenerate). The  $\Gamma_7^C$  and  $\Gamma_8^C$  bands shown above are the closest higher bands.

For  $\vec{k} \neq 0$  the  $\vec{k} \cdot \vec{p}$  interaction reduces the 4-fold degenerate of  $\Gamma_6^C$  into two 2-fold spin degenerate heavy (-) and light (+) hole valence bands. In the presence of a magnetic field, the spin degeneracies are removed. In the single-group representation the valence bands belong to  $\Gamma_4$  (in the notation of Ref. 14, this is called  $\Gamma_5$ ).



In P.B. treatment, the second term in  $\pi_{\ell\ell}$ , is ignored. Also the intermediate states  $u_{\ell_0}(\vec{r})$ , where  $\ell \neq j$  are those corresponding to the unperturbed Hamiltonian without spin-orbit interaction, that is, they have the symmetry of the single-group representations of the  $T_d$  group. Weiler<sup>8,9</sup> on the other hand considers  $u_{\ell_0}(\vec{r})$  belonging to the double-group representation of the  $T_d$  group and as a result she obtains additional parameters  $N_1, N_2, N_3$  and  $q$ , where  $q$  is the parameter found earlier by Luttinger.<sup>12</sup> For  $\vec{\pi}_{\ell\ell}$ , she also disregards the second term for  $\ell, \ell'$  outside the 8 bands under consideration. However, note that  $\vec{p}_{\ell\ell}$ , and  $\vec{\pi}_{\ell\ell}$ , have the same symmetry properties. From here on we give a brief account of her method and follow her results.

In Section B.3 the (effective-mass or so-called  $\vec{k} \cdot \vec{p}$ ) Hamiltonian of Eq.(2-1) is retained to second order in  $k$  and first order in  $H$  and obtained as an 8x8 matrix coupling the  $\Gamma_6^C(J=1/2)$  conduction band, the  $\Gamma_8^V(J=3/2)$  light and heavy hole bands, and the  $\Gamma_7^V(J=1/2)$  spin-orbit split-off valance band (see Figure II-1 for band diagram). The effect of other bands appears as coefficients in the 8x8 Hamiltonian matrix. In Section B.4, we give the simplified version of the Hamiltonian which is decoupled in two block-diagonal 4x4 matrices for the so-called a-set and b-set. This is the so-called quasi-Ge model Hamiltonian which affords us the ability to calculate numerically the energies of the valance and conduction bands in a magnetic field. The quasi-Ge model is

obtained from the full 8x8 Hamiltonian by neglecting a number of small terms which are proportional to the warping and asymmetry parameters. Weiler<sup>8,8</sup> has shown that when those terms are included they are responsible for cyclotron harmonic transitions which have been observed in InSb.

B. 3. The 8x8 Hamiltonian Matrix Using Double-Group Representation of  $T_d$

The basis functions  $u_{j_0}(\vec{r})$  used by Weiler<sup>8,9</sup> in the effective-mass Hamiltonian of Eq.(2-1) is given below in Table II-1.

TABLE II-1

a-set

$$|1\rangle = \psi_{1/2,1/2}^6 = S^\dagger$$

$$|3\rangle = \psi_{3/2,3/2}^8 = -\frac{i}{\sqrt{2}}(X + iY)^\dagger$$

$$|5\rangle = \psi_{3/2,-1/2}^8 = \frac{i}{\sqrt{6}}[(X - iY)^\dagger + 2Z^\dagger]$$

$$|7\rangle = \psi_{1/2,-1/2}^7 = -\frac{i}{\sqrt{3}}[(X - iY)^\dagger - Z^\dagger]$$

b-set

$$|2\rangle = \psi_{1/2,-1/2}^6 = S^\dagger$$

$$|6\rangle = \psi_{3/2,1/2}^8 = -\frac{i}{\sqrt{6}}[(X + iY)^\dagger - 2Z^\dagger]$$

$$|4\rangle = \psi_{3/2,-3/2}^8 = \frac{i}{\sqrt{2}}(X - iY)^\dagger$$

$$|8\rangle = \psi_{1/2,1/2}^7 = -\frac{i}{\sqrt{3}}[(X + iY)^\dagger + Z^\dagger]$$

In Table II-1 spatial functions  $X, Y, Z$  and the spin functions  $\uparrow$  and  $\downarrow$  are those used by Kane,<sup>11</sup> for the zero magnetic field case. The superscript on  $\psi$  indicates which double-group representation of  $T_d$   $\psi$  belongs to, and the subscripts give  $J$  and  $M_J$ , the quantum numbers for the total angular momentum and its  $z$  component, respectively.

As mentioned in B.1 of this Chapter Weiler<sup>8,9</sup> considers all of the matrix elements of  $\vec{k}$  and  $\vec{k} \times \vec{k}$  among  $\Gamma_6^C, \Gamma_8^V$ , and  $\Gamma_7^V$  (Figure II-1). Some of these couplings involve only these subset of bands, and some involve higher bands with  $\Gamma_6, \Gamma_8$ , and  $\Gamma_7$  symmetry as intermediate states. Table II-2 summarizes all of the real independent parameters in this manner (same as Table II-2 of Ref. 8 and Table I of Ref. 9). The  $\Gamma_8 \times \Gamma_8$  parameters  $\gamma_1, \gamma_2, \gamma_3, \kappa$  and  $q$  are defined in Ref. 12. The  $\Gamma_7 \times \Gamma_8$  parameters are independent of the  $\Gamma_8 \times \Gamma_8$  parameters, but are expected to be very close to them. Explicit expressions for these band parameters will be given in Appendix B. Table II-3 of Ref. 8, (same as Table II of Ref. 9) gives the  $8 \times 8$   $\vec{k} \cdot \vec{p}$  Hamiltonian to second order in  $k$  and first order in  $H$  and will not be reproduced here.

#### B. 4. Quasi-Ge Model in a Magnetic Field

For a magnetic field  $H$  in the direction defined by the spherical polar angles  $\theta$  and  $\phi$ , with respect to the principal symmetry axes  $(x, y, z)$ , a coordinate transformation is performed

TABLE II-2 Parameters of the  $\vec{k} \cdot \vec{p}$  Hamiltonian among the  $\Gamma_8$ ,  $\Gamma_7$  and  $\Gamma_6$  band-edge states. (After Ref. 8).

$f(\vec{k})$	$k_x$	$\vec{k}^2$	$2k_z^2 - k_x^2 - k_y^2$	$\{k_y, k_z\}$	$i[k_y, k_z]$
	$k_y$		$\sqrt{3}(k_x^2 - k_y^2)$	$\{k_z, k_x\}$	$i[k_z, k_x]$
	$k_z$			$\{k_x, k_y\}$	$i[k_x, k_y]$
$\langle \Gamma_6^C   f(\vec{k})   \Gamma_6^C \rangle$		F			$N_1$
$\langle \Gamma_8^V   f(\vec{k})   \Gamma_8^V \rangle$	C	$\gamma_1$	$\gamma_2$	$\gamma_3$	$\kappa, \rho$
$\langle \Gamma_7^V   f(\vec{k})   \Gamma_7^V \rangle$		$\gamma_1'$			$\kappa'$
$\langle \Gamma_6^C   f(\vec{k})   \Gamma_8^V \rangle$	P		$N_2$	G	$N_3$
$\langle \Gamma_6^C   f(\vec{k})   \Gamma_7^V \rangle$	P'			G'	
$\langle \Gamma_7^V   f(\vec{k})   \Gamma_8^V \rangle$	C'		$\gamma_2'$	$\gamma_3'$	$\kappa''$

so that in the new-coordinate system (1,2,3), the magnetic field would be along the 3-axis. The corresponding rotation of the basis states results in a transformation of the  $\vec{k} \cdot \vec{p}$  Hamiltonian according to  $\mathcal{H}(\theta, \phi) = U^\dagger \mathcal{H} U$  with  $U$  given in Table II-4 of Ref. 8.

Note that with  $H$  along the 3-axis, i.e.,  $\vec{H} = H(0,0,1)$ ,  $\vec{A}$  can be chosen such that  $\vec{A} = \frac{1}{2}H(-\vec{r}_2, \vec{r}_1, 0)$  (Landau gauge). Then, since  $\hbar \vec{k} = [\vec{p} + (e/c)\vec{A}]$ , we have  $k_1 = (1/\hbar)[p_1 - (\frac{eH}{2c})r_2]$ , and  $k_2 = (1/\hbar)[p_2 - (\frac{eH}{2c})r_1]$ . Since  $[r_\alpha, p_\beta] = i\hbar \delta_{\alpha\beta}$  it is recognized that if one defines  $a \equiv \frac{\lambda}{\sqrt{2}}(k_1 - ik_2)$  and  $a^+ \equiv \frac{\lambda}{\sqrt{2}}(k_1 + ik_2)$  with  $\lambda \equiv (\hbar c/eH)^{1/2}$  then one obtains

$$[a, a^+] = 1 \quad (2-6)$$

$a^+$  and  $a$  are thus recognized as the raising and lowering operators for the harmonic oscillator wave functions with  $a^+ \phi_n = \sqrt{n+1} \phi_{n+1}$ ,  $a \phi_n = \sqrt{n} \phi_{n-1}$ , and  $a^+ a \phi_n = n \phi_n$ . The operators  $k_1$  and  $k_2$  can then be expressed as

$$k_1 = \frac{1}{\lambda\sqrt{2}} (a + a^+), \quad (2-7a)$$

$$k_2 = \frac{i}{\lambda\sqrt{2}} (a - a^+) \quad (2-7b)$$

$$k_3 \equiv k_H \quad (2-7c)$$

in the 8x8 Hamiltonian of Refs. 8 and 9.

Next in the transformed Hamiltonian  $\mathcal{H}(\theta, \phi)$  if one neglects terms proportional to  $k_H$ ,  $q, C, G, N_2$  and  $N_3$  and most terms proportional to the warping parameter  $\mu \equiv \frac{1}{2}(\gamma_3 - \gamma_2)$  one gets the 8x8 Hamiltonian separated into two block diagonal 4x4 Hamiltonians corresponding to the a-set and the b-set, i.e.,

$$\mathcal{H}(\theta, \phi) \approx \begin{bmatrix} \mathcal{H}_a & 0 \\ 0 & \mathcal{H}_b \end{bmatrix}_{(8 \times 8)} \quad (2-8)$$

where  $\mathcal{H}_a$  and  $\mathcal{H}_b$  are called the quasi-Ge model Hamiltonians given here in Table II-3 where

$$\gamma' = \gamma_3 + (\gamma_2 - \gamma_3)f(\theta, \phi) \quad (2-9a)$$

$$\gamma'' = \frac{1}{3}\gamma_2 + \frac{2}{3}\gamma_3 + \frac{1}{6}(\gamma_2 - \gamma_3)f(\theta, \phi) \quad (2-9b)$$

with

$$f(\theta, \phi) = \left(\frac{3 \cos^2 \theta - 1}{2}\right)^2 + \frac{3}{4} \cos^2 2\phi \sin^4 \theta \quad (2-9c)$$

For  $\phi=45^\circ$ , i.e., H in the  $(1\bar{1}0)$  plane  $\bar{q}_1$  and  $\bar{q}_2$  are given as:

TABLE II-3 The Quasi-Ge Model Hamiltonian

$$\mathcal{H}_a = \begin{array}{cccc}
 |1\rangle & |3\rangle & |5\rangle & |7\rangle \\
 \left[ \begin{array}{cccc}
 E_g + 2\beta H[F(2a^+a+1) + N_1 + (a^+a+1)] & (\beta H E_p)^{1/2} a^+ & -(\frac{1}{3}\beta H E_p)^{1/2} a & (\frac{2}{3}\beta H E_p)^{1/2} a \\
 (\beta H E_p)^{1/2} a & -\beta H[(\gamma_1 + \gamma')(2a^+a+1) + 3\kappa + \bar{q}_1] & 2\sqrt{3} \gamma'' \beta H a^2 & -2\sqrt{6} \gamma'' \beta H a^2 \\
 -(\frac{1}{3}\beta H E_p)^{1/2} a^+ & 2\sqrt{3} \gamma'' \beta H a^{+2} & -\beta H[(\gamma_1 - \gamma')(2a^+a+1) - \kappa + \bar{q}_5] & \sqrt{2}\beta H[\gamma'(2a^+a+1) - \kappa - 1] \\
 (\frac{2}{3}\beta H E_p)^{1/2} a^+ & -2\sqrt{6} \gamma'' \beta H a^{+2} & \sqrt{2}\beta H[\gamma'(2a^+a+1) - \kappa - 1] & -\Delta - \beta H[\gamma_1(2a^+a+1) - 2\kappa - 1]
 \end{array} \right] & \begin{array}{l} |1\rangle \\ |3\rangle \\ |5\rangle \\ |7\rangle \end{array} \\
 \\
 |2\rangle & |6\rangle & |4\rangle & |8\rangle \\
 \left[ \begin{array}{cccc}
 E_g + 2\beta H[F(2a^+a+1) - N_1 + a^+a] & (\frac{1}{3}\beta H E_p)^{1/2} a^+ & -(\beta H E_p)^{1/2} a & (\frac{2}{3}\beta H E_p)^{1/2} a^+ \\
 (\frac{1}{3}\beta H E_p)^{1/2} a & -\beta H[(\gamma_1 - \gamma')(2a^+a+1) + \kappa - \bar{q}_5] & 2\sqrt{3} \gamma'' \beta H a^2 & -\sqrt{2} \beta H[\gamma'(2a^+a+1) + \kappa + 1] \\
 -(\beta H E_p)^{1/2} a^+ & 2\sqrt{3} \gamma'' \beta H a^{+2} & -\beta H[(\gamma_1 + \gamma')(2a^+a+1) - 3\kappa - \bar{q}_1] & 2\sqrt{6} \gamma'' \beta H a^{+2} \\
 (\frac{2}{3}\beta H E_p)^{1/2} a & -\sqrt{2} \beta H[\gamma'(2a^+a+1) + \kappa + 1] & 2\sqrt{6} \gamma'' \beta H a^2 & -\Delta - \beta H[\gamma_1(2a^+a+1) + 2\kappa + 1]
 \end{array} \right] & \begin{array}{l} |2\rangle \\ |6\rangle \\ |4\rangle \\ |8\rangle \end{array}
 \end{array}$$

$$\bar{q}_1 = \frac{3}{4} q(3 \cos^4 \theta - 2 \cos^2 \theta + 8) \quad (2-10a)$$

$$\bar{q}_5 = \frac{1}{4} q(27 \cos^4 \theta - 18 \cos^2 \theta - 10). \quad (2-10b)$$

The operators  $a$  and  $a^+$  are given by

$$a = \left(\frac{2eH}{\hbar c}\right)^{-1/2} (k_1 + ik_2), \quad (2-11a)$$

$$a^+ = \left(\frac{2eH}{\hbar c}\right)^{-1/2} (k_1 - ik_2) \quad (2-11b)$$

and  $\beta \equiv \mu_B \equiv (e\hbar/2mc) \equiv \text{Bohr magneton} \quad (2-11c)$

$$E_p \equiv 2mP^2/\hbar^2 \quad (2-12)$$

The Hamiltonians in Table II-3 are equivalent to those of P.B.<sup>7</sup> with the following corrections:

- 1) The parameter  $N_1$ , which gives the effect of intermediate states on the  $g$ -factor of the conduction band, as well as diagonal terms proportional to  $q$ , are included here.
- 2) In Eq.(10) of Ref. 7, for the (3,7) and (7,3) matrix elements,  $\gamma'$  should be replaced by  $-\gamma''$ .
- 3) In Eq.(11) of Ref. 7, for the (4,8) and (8,4) matrix elements,  $\gamma'$  should be replaced by  $\gamma''$ .

In the quasi-Ge model one then has to solve these two Schrödinger equations for the  $a$ -set and the  $b$ -set.

$$\mathcal{H}_a |a\rangle = E_a |a\rangle \quad (2-13a)$$

$$\mathcal{H}_b |b\rangle = E_b |b\rangle \quad (2-13b)$$

The solutions are of the following form.

$$|a\rangle = \begin{bmatrix} a_1^n \phi_n \\ a_3^n \phi_{n-1} \\ a_5^n \phi_{n+1} \\ a_7^n \phi_{n+1} \end{bmatrix}, \quad |b\rangle = \begin{bmatrix} b_2^n \phi_n \\ b_6^n \phi_{n-1} \\ b_4^n \phi_{n+1} \\ b_8^n \phi_{n-1} \end{bmatrix} \quad (2-14a)$$

$$(2-14b)$$

where  $n$  is an integer and  $n \geq -1$ .

Here  $\phi_n$  is the harmonic oscillator wave function so that  $a^+ \phi_n = \sqrt{n+1} \phi_{n+1}$  and  $a \phi_n = \sqrt{n} \phi_{n-1}$ . The coefficients  $a_j^n$  and  $b_j^n$  are zero for those values of  $n$  which make the subscript of  $\phi$  negative: i.e.,

$$a_{-1}^{-1} = a_{-3}^{-1} = a_3^0 = b_{-2}^{-1} = b_6^0 = b_{-6}^{-1} = b_{-8}^{-1} = b_8^0 = 0$$

For each integer  $n \geq 1$  the two 4x4 Hamiltonians give eight independent solutions:  $|a^c(n)\rangle$ ,  $|b^c(n)\rangle$ ,  $|a^-(n)\rangle$ ,  $|b^-(n)\rangle$ ,  $|a^+(n)\rangle$ ,  $|b^+(n)\rangle$ ,  $|a^{so}(n)\rangle$ ,  $|b^{so}(n)\rangle$ , where "c" refers to the conduction band, "-" and "+" to the heavy and light hole valence bands respectively, and "so" to the spin-orbit split-off band. In fact with eigen-vectors of the form in Eqs.(2-14) the  $a$ ,  $a^+$ ,  $a^2$ , and  $a^{+2}$  operators in matrices of Table II-3 can be replaced by

expressions involving  $n$ , more explicitly:  $a^2$  and  $a^{+2}$  are replaced by  $[n(n+1)]^{1/2}$ , and

$$\begin{aligned}
 & (n) \quad \text{in } (1,1), (2,2) \\
 a^+ a \rightarrow & (n-1) \text{ in } (3,3), (6,6), (8,8), (6,8), (8,6) \\
 & (n+1) \text{ in } (5,5), (7,7), (5,7), (7,5), (4,4) \\
 a \rightarrow & (n+1)^{1/2} \text{ in } (1,5), (1,7), (2,4) \\
 & (n)^{1/2} \text{ in } (3,1), (6,2), (8,2) \\
 a^+ \rightarrow & (n+1)^{1/2} \text{ in } (5,1), (7,1), (4,2) \\
 & (n)^{1/2} \text{ in } (1,3), (2,6), (2,8)
 \end{aligned}$$

giving the two 4x4 quasi-Ge model Hamiltonian matrices in terms of  $n$ . One can then use a computer to determine eigenvalues for Eqs.(2-13) as well as eigen-vectors (i.e., values for  $a_n$  and  $b_n$ 's), for a given set of band parameters and arbitrary  $n$ .

### C. Some Results of the Quasi-Ge Model

Reference 6 gives explicit expressions for the determinantal equations for the eigenvalue problem of Eqs.(2-13); this is given in Eq.(83), where the terms involved are defined in Eqs.(81) and (82) for the a-set and the b-set respectively. In Eq.(81) one should read  $F=-[6n(n+1)]^{1/2}\gamma$ ". In this treatment  $N_1$  and  $q$  are ignored. The eigenvalues ( $E_a$  and  $E_b$  in our

notation) are expanded in a power series in  $s$  ( $s \equiv 2\beta H$ ) and expressions are obtained for the eigen-energies up to second-order in  $H$ .

### C. 1. Energies Up to First Order in H

The conduction band energies to first order in  $H$  are

$$\left. \begin{array}{l} E[a^c(n)] \\ E[b^c(n)] \end{array} \right\} = E_g + (n + \frac{1}{2}) \hbar \omega_c \pm \frac{1}{2} g_c \beta H \quad (2-15)$$

where  $\omega_c$ , the cyclotron frequency,  $m_c$  the effective mass, and  $g_c$  the  $g$ -factor, are for the conduction band and they are given as follows:

$$\omega_c = eH/m_c c \quad (2-16)$$

$$\frac{m}{m_c} \equiv 1 + \frac{1}{3} E_p \left( \frac{2}{E_g} + \frac{1}{E_g + \Delta} \right) + 2F \quad (2-17)$$

$$g_c \equiv 2 - \frac{2}{3} E_p \left( \frac{1}{E_g} - \frac{1}{E_g + \Delta} \right) + 4N_1 \quad (2-18)$$

$$= 2 \left[ 1 - \frac{E_p}{3E_g} \cdot \frac{\Delta}{E_g + \Delta} \right] + 4N_1 \quad (2-18a)$$

which include the higher band contributions  $F$  and  $N_1$ . These contribution have been considered earlier by Groves<sup>15</sup> and more recently by Hermann and Weisbuch<sup>16</sup> (see Appendix B). The valence band energies to first order are<sup>8</sup> (+ for light hole, - for heavy hole;  $n \geq 1$  for heavy holes and  $n \geq -1$  for light holes).

$$E[a^\pm(n)] = -2\beta H \left\{ (n+\frac{1}{2})\gamma_1^L - \gamma'^L + \frac{1}{2}\kappa^L + (\frac{5}{8}+f)q \right. \\ \left. \pm \sqrt{[\gamma_1^L - (n+\frac{1}{2})\gamma'^L - \kappa^L - \frac{1}{2}(\frac{9}{2}-f)q]^2 + 3n(n+1)(\gamma''^L)^2} \right\} \quad (2-19)$$

$$E[b^\pm(n)] = -2\beta H \left\{ (n+\frac{1}{2})\gamma_1^L + \gamma'^L - \frac{1}{2}\kappa^L - (\frac{5}{8}+f)q \right. \\ \left. \pm \sqrt{[\gamma_1^L + (n+\frac{1}{2})\gamma'^L - \kappa^L - \frac{1}{2}(\frac{9}{2}-f)q]^2 + 3n(n+1)(\gamma''^L)^2} \right\} \quad (2-20)$$

where  $f \equiv f(\theta, \phi)$  and  $\gamma_1^L, \gamma'^L, \text{ etc.}$  are the Luttinger<sup>12</sup> parameters:

$$\gamma_1^L \equiv \frac{1}{3}(E_p/E_g) + \gamma_1 \quad (2-21a)$$

$$\gamma'^L \equiv \frac{1}{6}(E_p/E_g) + \gamma' \quad (2-21b)$$

$$\gamma''^L \equiv \frac{1}{6}(E_p/E_g) + \gamma'' \quad (2-21c)$$

$$\kappa^L \equiv \frac{1}{6}(E_p/E_g) + \kappa \quad (2-21d)$$

For  $n=-1$  and  $0$ , and assuming  $q=0$

$$E[a^+(-1)] = -\beta H [\gamma_1^L - \gamma'^L - \kappa^L] \quad (2-22a)$$

$$E[a^+(0)] = -\beta H [3\gamma_1^L - 3\gamma'^L - \kappa^L] \quad (2-22b)$$

$$E[b^+(-1)] = -\beta H [\gamma_1^L + \gamma'^L - 3\kappa^L] \quad (2-22c)$$

$$E[b^+(0)] = -\beta H [3\gamma_1^L + 3\gamma'^L - 3\kappa^L] \quad (2-22d)$$

For large  $n$ , Eqs. (2-19) and (2-20) give

$$E[a^{\pm}(n)] - E[a^{\pm}(n+1)] \approx \left(\frac{m}{m_{\pm}}\right) \cdot 2\beta H > 0 \quad (2-23)$$

and similarly for the b-set. Here the effective masses for the heavy (-) and the light (+) hole bands are given by

$$\frac{m}{m_{\pm}} = \gamma_1^L \pm [(\gamma_1^L)^2 + 3(\gamma_2^L)^2]^{1/2} \quad (2-24)$$

For  $E_p/E_g \gg \gamma_1, \gamma_2$  this gives

$$\frac{m}{m_+} \approx \frac{2}{3} \frac{E_p}{E_g} + \gamma_1 + \frac{1}{2}(\gamma_1 + 3\gamma_2) \quad (2-25a)$$

$$\frac{m}{m_-} \approx \gamma_1 - \frac{1}{2}(\gamma_1 + 3\gamma_2) \quad (2-25b)$$

which shows that the light hole band is nearly the mirror image of the conduction band, and the heavy hole mass has a large effective mass  $\sim \gamma_1^{-1}$

For the spin-orbit split-off band, to first order in H

$$E[a^{SO}(n)] = -\Delta - (n + \frac{3}{2}) \left[ \frac{m}{m_{SO}} + \frac{1}{4}g_{SO} \right] 2\beta H, \text{ with } n = -1, 0, 1, \dots \quad (2-26a)$$

$$E[b^{SO}(n)] = -\Delta - (n - \frac{1}{2}) \left[ \frac{m}{m_{SO}} - \frac{1}{4}g_{SO} \right] 2\beta H, \text{ with } n = 1, 2, 3, \dots \quad (2-26b)$$

$$\frac{m}{m_{SO}} = \gamma_1^L - \frac{E_p}{3} \left[ \frac{1}{E_g} - \frac{1}{E_g + \Delta} \right] \quad (2-27a)$$

$$= \gamma_1 + \frac{E_p}{3(E_g + \Delta)} \quad (2-27b)$$

and

$$g_{s0} = -2 \left[ 2\kappa^L + 1 - \frac{E_p}{3E_g} \cdot \frac{\Delta}{E_g + \Delta} \right] \quad (2-28)$$

which gives

$$g_c + g_{s0} = -4(\kappa^L - N_1) \quad (2-29)$$

It turns out that  $N_1$  is very small (Appendix B, and Ch.IV), therefore,

$$g_c + g_{s0} \approx -4\kappa^L \quad (2-30)$$

### C. 2. Energies Up to Second Order in H

We now consider the corrections to the energies, second-order in  $H$ . For this purpose, we could follow the procedure of Ref.6 and use Eq.(102). From this equation one can find correction to the conduction band energy. For simplicity one can ignore the effect of higher bands and obtain Kane's formula,<sup>11</sup> namely set  $F=0$ ,  $\gamma_1=-1$ ,  $\gamma_2=\gamma_3=0$ ,  $\kappa=-\frac{1}{3}$ . Then for the average conduction band a and b series energies in the units of  $(2\beta H)^2$  Ref.6 finds the following second-order correction.

$$\mathcal{E}_2^c = (n+\frac{1}{2})^{1/2} \left( \frac{m}{m_c} - 1 \right)^2 \left( \frac{3E_g + 4\Delta + 2\Delta^2/E_g}{(E_g + \Delta)(3E_g + 2\Delta)} \right) \quad (2-31)$$

[See Eq.(110) of Ref. 6 for example]. Note that in this formula

$\frac{m}{m_c}$  is given by Eq.(2-17) but with  $F=0$ . This result is in agreement with Vrehan.<sup>17</sup> He started with Kane's determinantal equation, i.e.,

$$E'[(E'-E_g)(E')(E'+\Delta) - k^2 P^2 (E'+\frac{2}{3}\Delta)] = 0 \quad (2-32)$$

where

$$E' = E(k) - \frac{\hbar^2 k^2}{2m} \quad (2-33)$$

and from Eq.(2-12)

$$P^2 = \frac{\hbar^2}{2m} E_p \quad (2-34)$$

For the conduction band, keeping only terms up to  $k^4$ , Vrehan obtained, again with  $F=0$ ,

$$E_c = E_g + \left(\frac{m}{m_c}\right) \frac{\hbar^2 k^2}{2m} - \left(\frac{m}{m_c} - 1\right)^2 \left(\frac{\hbar^2 k^2}{2m}\right)^2 \left[ \frac{3E_g + 4\Delta + 2\Delta^2/E_g}{(E_g + \Delta)(3E_g + 2\Delta)} \right] \quad (2-35)$$

One can then make the following substitution

$$\frac{\hbar^2 k^2}{2m} \rightarrow (n + \frac{1}{2})(2\beta\hbar) \quad (2-36)$$

to obtain the expression for the average energy of the conduction band a and b series in agreement with Eq.(2-31).

Johnson,<sup>18</sup> starts with Eq.(2-32) and rearranges terms to obtain

$$E'(E'-E_g) = k^2 P^2 \left( \frac{E'+\frac{2}{3}\Delta}{E'+\Delta} \right) \quad (2-37)$$

This yields

$$E_c = \frac{1}{2}E_g + \frac{\hbar^2 k^2}{2m} + \frac{1}{2} E_g \left[ 1 + 4 \frac{\hbar^2 k^2}{2m_c} \cdot \frac{f_1(E')}{E_g} \right]^{1/2} \quad (2-38)$$

where

$$f_1(E') = \frac{E_g + \Delta}{E_g + \frac{2}{3}\Delta} \cdot \frac{E' + \frac{2}{3}\Delta}{E' + \Delta} \quad (2-39)$$

Comparing this with Eqs.(41) and (51) of Ref. 18, one see that in Ref. 18,  $f_1(E_c)$  is used instead of  $f_1(E')$ . Again when one keeps terms up to  $k^4$ , one can recover (2-35). In all of the above treatments the higher band contributions including F is ignored. We would like to keep F nonzero. We start from Kane's determinantal Equation,<sup>11</sup> this time including F, the higher-bands contribution to the conduction band effective mass. Kane's determinantal equation becomes:

$$E'[(E'' - E_g)(E'')(E' + \Delta) - \frac{\hbar^2 k^2}{2m} E_p(E' + \frac{2}{3}\Delta)] = 0 \quad (2-40)$$

Here

$$E'' = E' - \left( \frac{\hbar^2 k^2}{2m} \right) 2F \quad (2-41a)$$

$$E' = E - \frac{\hbar^2 k^2}{2m} \quad (2-41b)$$

For the conduction band let us expand E up to  $k^4$ , i.e.,

$$E = E_g + (X+1) \frac{\hbar^2 k^2}{2m} + Y \left( \frac{\hbar^2 k^2}{2m} \right)^2 \quad (2-42)$$

we then have to find X and Y. Let us define

$$\lambda \equiv \frac{\hbar^2 k^2}{2m} \quad (2-43)$$

We now substitute (2-42) in (2-40) using (2-41). This gives the following equation, correct to  $\lambda^2$ :

$$\begin{aligned} \lambda[(X-2F)+Y\lambda][E_g+X\lambda + Y\lambda^2][(E_g+\Delta)+X\lambda + Y\lambda^2] \\ -\lambda E_p[(E_g+\frac{2}{3}\Delta) + X\lambda + Y\lambda^2] = 0 \end{aligned}$$

For this to hold for arbitrary k (and for terms up to  $k^4$ ) we require the coefficients of  $k^2$  and  $k^4$ , i.e., coefficients of  $\lambda$  and  $\lambda^2$  to be identically zero: this gives

$$\left\{ \begin{aligned} (X-2F)E_g(E_g+\Delta) - E_p(E_g+\frac{2}{3}\Delta) &= 0 & (2-44) \\ (X-2F)[E_g + X(E_g+\Delta)] + Y E_g(E_g+\Delta) - E_p X &= 0 & (2-45) \end{aligned} \right.$$

Equation (2-44) gives:

$$X-2F = \frac{E_p(E_g+\frac{2}{3}\Delta)}{E_g(E_g+\Delta)} \quad (2-46)$$

or

$$X = \frac{E_p}{3} \left( \frac{2}{E_g} + \frac{1}{E_g+\Delta} \right) + 2F \quad (2-47)$$

We immediately recognize that the coefficient multiplying  $k^2$  in Eq.(2-42) is

$$(X+1) \equiv \frac{m}{m_c} \quad (2-48)$$

Where  $\frac{m}{m_c}$  is given by Eq.(2-17), and this is not surprising. As for  $Y$ , Eq.(2-45) gives

$$Y = -X \left[ \frac{(X-2F)(2E_g + \Delta) - E_p}{E_g(E_g + \Delta)} \right] \quad (2-49)$$

Using Eq.(2-46) this yields:

$$Y = -X \frac{E_p (3E_g + 2\Delta)}{3E_g(E_g + \Delta)} \cdot \left\{ \frac{3E_g + 4\Delta + 2\Delta^2/E_g}{(E_g + \Delta)(3E_g + 2\Delta)} \right\} \quad (2-50)$$

Using Eqs. (2-48) and (2-17) and this gives

$$Y = -\left(\frac{m}{m_c} - 1\right) \left(\frac{m}{m_c} - 1 - 2F\right) \left\{ \frac{3E_g + 4\Delta + 2\Delta^2/E_g}{(E_g + \Delta)(3E_g + 2\Delta)} \right\} \quad (2-51)$$

Thus

$$E_c = E_g + \left(\frac{m}{m_c}\right) \frac{\hbar^2 k^2}{2m} - \left(\frac{m}{m_c} - 1\right) \left(\frac{m}{m_c} - 1 - 2F\right) \left(\frac{\hbar^2 k^2}{2m}\right) \times \left\{ \frac{3E_g + 4\Delta + 2\Delta^2/E_g}{(E_g + \Delta)(3E_g + 2\Delta)} \right\} \quad (2-52)$$

In a magnetic field, the average energy of a and b series is obtained

below, using the substitution (2-36) in Eq.(2-52)

$$E_c = E_g + (n+\frac{1}{2})\left(\frac{m}{m_c}\right)(2\beta H) - (n+\frac{1}{2})^2 \left(\frac{m}{m_c} - 1\right)\left(\frac{m}{m_c} - 1 - 2F\right) \left(\frac{3E_g + 4\Delta + 2\Delta^2/E_g}{(E_g + \Delta)(3E_g + 2\Delta)}\right) (2\beta H)^2 \quad (2-53)$$

In Eqs.(2-52) and (2-53),  $\frac{m}{m_c}$  is given by Eq.(2-17) which includes F. Here  $m_c$  is the effective mass at the bottom of the conduction band. For F=0, our result is in agreement with that of Refs. 6, 17 and 18. However, Eqs.(2-52) and (2-53) bring out a feature hidden in the above references where F=0 is assumed. Note that in the nonparabolic term, proportional to  $k^4$  or  $H^2$ ,  $(\frac{m}{m_c} - 1 - 2F)$  is proportional to  $E_p$ . Therefore presumably although different values of  $E_p$  and F can be adjusted to give the same value for  $m_c$  for the parabolic term (proportional to  $k^2$  or H), the nonparabolic term is different for different values of F. Would this help narrow down the range of acceptable values for F? To answer this, the effect of  $\gamma_1, \gamma_2, \gamma_3$ , and  $\kappa$  should also be included (see Appendix C). In Chapter IV this question will be considered in some detail.

#### D. Magneto-optical Transitions: Selection Rules

Magneto-optical transitions come about from the coupling among the eigenstates of Eqs.(2-13) which have the form given in Eqs.(2-14), via the optical field Hamiltonian  $\mathcal{H}'(\omega)$ , at circular frequency  $\omega$ .

The strongest allowed one photon optical transitions among these eigenstates are those transitions which are proportional to the

interband matrix element  $P$ . For these transitions, the matrix elements containing terms of the type  $\vec{k}P$  in the full  $8 \times 8$   $\vec{k} \cdot \vec{p}$  Hamiltonian of Refs. 8 and 9 are replaced as follows:

$$\vec{k}P, \vec{k}P' \rightarrow [\vec{k} + (e/\hbar c)\vec{A}']P \quad (2-54)$$

where  $P$  is given by Eq.(2-34) in terms of  $E_p$ , and  $\vec{A}'$  is the vector potential of the radiation field in the radiation gauge. In the  $8 \times 8$   $\vec{k} \cdot \vec{p}$  Hamiltonian (Table II of Ref. 9) there are two types of terms proportional to  $P$  (and  $P'$  with  $P' \sim P$ ). The first type couples the states of the a-set to those in the a-set; or the states in the b-set to those in the b-set. The second type couples the states of the a-set to those of the b-set. The latter type of terms appear in the following matrix elements: (1,6), (1,8), (2,5), (2,7), (6,1), (8,1), (5,2) and (7,2). These terms are proportional to  $PK_3$  (or  $P'K_3$ ;  $P' \sim P$ ). For the quasi-Ge model, we recall that  $C, G, N_2, N_3$ , and most terms proportional to  $(\gamma_3 - \gamma_2)$  as well as  $k_3 \equiv k_H$  were set equal to zero. However, in the presence of the radiation field according to Eq.(2-54)  $k_3 \rightarrow k_3 + (e/\hbar c)A'_3$ , and hence even with  $k_3 = 0$ ,  $(e/\hbar c)A'_3$  survives. As a result, the presence of radiation field can cause coupling between the a-set and the b-set states as well.

The matrix elements for the optical transitions are<sup>8</sup>

$$\langle a(n') | \mathcal{H}_0(\omega) | a(n) \rangle = \quad (2-55a)$$

$$\frac{eE}{\omega} \left( \frac{E_p}{6m} \right)^{1/2} \left\{ [\sqrt{3} a_3^{n'} a_1^n - a_1^{n'} (a_5^n - \sqrt{2} a_7^n)] \hat{\epsilon}_- \delta_{n', n+1} + [n \leftrightarrow n'] \hat{\epsilon}_+ \delta_{n', n-1} \right\}$$

$$\langle b(n') | \mathcal{H}'(\omega) | b(n) \rangle = \quad (2-55b)$$

$$\frac{eE}{\omega} \left( \frac{E_p}{6m} \right)^{1/2} \left[ (b_6^{n'} + \sqrt{2} b_8^{n'}) b_2^n - \sqrt{3} b_2^{n'} b_4^n \right] \hat{\epsilon}_- \delta_{n', n+1} + [n \leftrightarrow n'] \hat{\epsilon}_+ \delta_{n', n-1}$$

$$\langle b(n') | \mathcal{H}'(\omega) | a(n) \rangle = \quad (2-55c)$$

$$-\frac{eE}{\omega} \left( \frac{E_p}{6m} \right)^{1/2} [b_2^{n'} (\sqrt{2} a_5^n + a_7^n) + (\sqrt{2} b_6^{n'} - b_8^{n'}) a_1^n] \hat{\epsilon}_3 \delta_{n', n+1}$$

Here  $E$  is the optical electric field, and  $\hat{\epsilon}_{\pm} \equiv (\hat{\epsilon}_1 \pm i\hat{\epsilon}_2)/\sqrt{2}$ . The unit polarization vectors  $\hat{\epsilon}_+$  and  $\hat{\epsilon}_-$  correspond respectively to right and left circular polarization (RCP, LCP) transverse to  $\vec{H}$  and  $\hat{\epsilon}_3$  is the unit polarization vector parallel to  $\vec{H}$  ( $\vec{E} \parallel \vec{H}$ , or  $\hat{\epsilon}$  polarization). The one photon optical selection rules are then

$$\vec{k} \parallel \vec{H} \quad \begin{cases} \sigma_L(\text{LCP}) & a(n) \rightarrow a(n+1) \text{ and } b(n) \rightarrow b(n+1) \\ \sigma_R(\text{RCP}) & a(n) \rightarrow a(n-1) \text{ and } b(n) \rightarrow b(n-1) \end{cases} \quad (2-56)$$

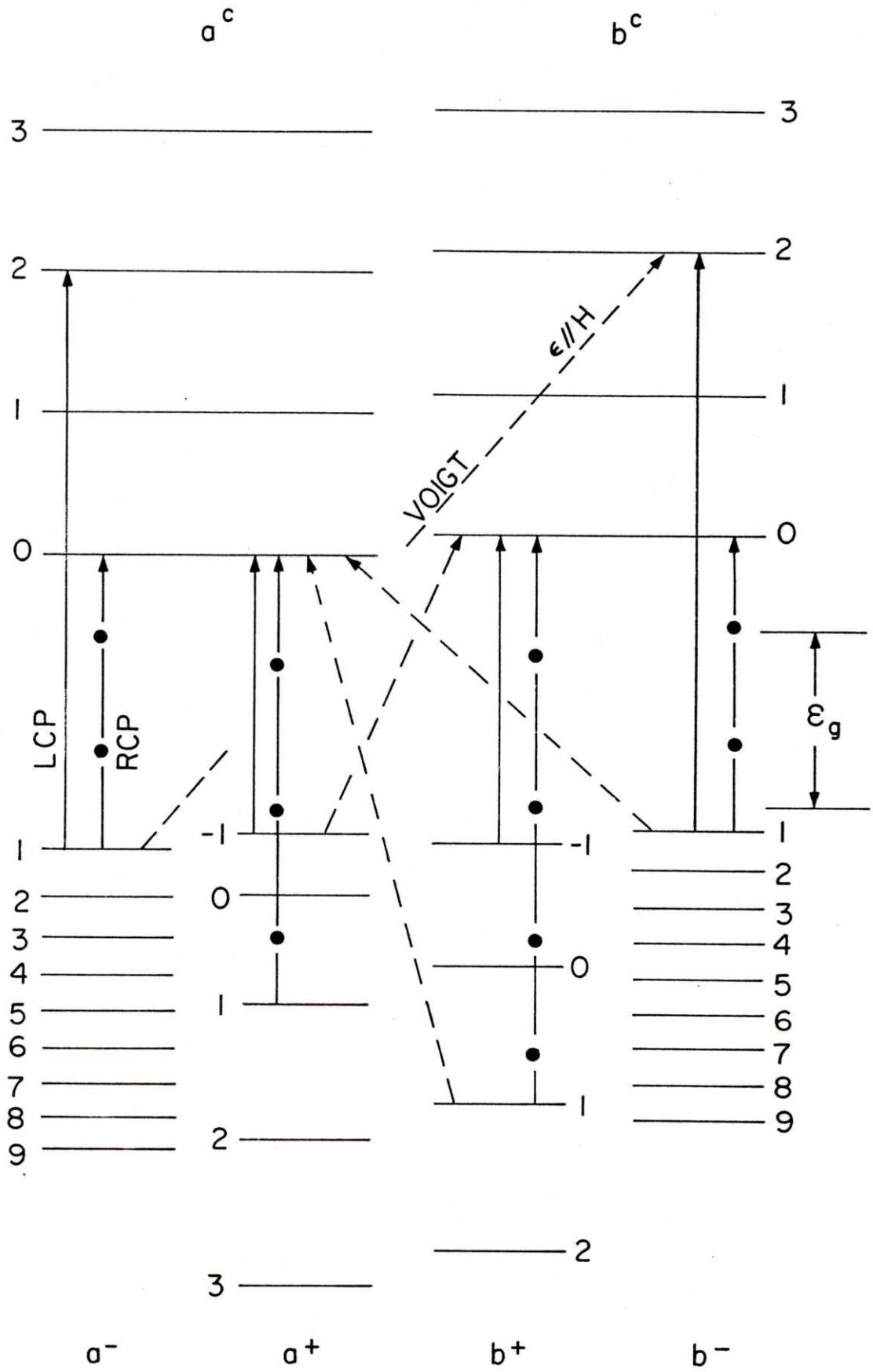
$$\vec{k} \perp \vec{H} \quad \begin{cases} \pi(\text{E} \parallel \text{H}) & a(n) \rightarrow b(n+1) \text{ and } b(n) \rightarrow a(n-1) \\ \hat{\epsilon} \perp \vec{H} & a(n) \rightarrow a(n+1), a(n-1) \\ & b(n) \rightarrow b(n+1), b(n-1) \end{cases}$$

Intuitively, if one recalls that generally speaking "a" is associated with spin up and "b" with spin down electron, and  $n$  with the orbital angular momentum of the electron, then the selection rules above could be considered as a statement of conservation of angular momentum for the "light and electron" system.

Figure II-2 shows schematically the Landau levels for the

conduction band a-set and b-set as well as the light-hole (+) and the heavy hole (-) a-set and b-set. The lowest-energy allowed interband magneto-optical transitions for the Voigt  $\vec{E} \parallel \vec{H}$  and for the Faraday (RCP and LCP) configurations are shown by arrows. It is seen from the selection rules that the first two transitions in the LCP originate from the light-hole bands.

FIGURE II-2 The Landau levels for the conduction band and the light-hole and heavy-hole valence bands. The value of the Landau quantum number for each level is shown. The lowest-energy allowed interband transitions for the Faraday configuration (RCP and LCP) and for the Voigt configuration are indicated by the arrows.  $\epsilon_g$  is the same as  $E_g$  in our notation. (After Reine et al.<sup>19</sup>)



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## CHAPTER III

### MAGNETOABSORPTION EXPERIMENTS

In this chapter, we describe the details of our experiments on  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$ , describing the samples in Section A and the experimental setup and data acquisition system in Section B. In Section C we present some magnetotransmission spectra  $T(H)/T(0)$  vs. photon energy, where  $T(H)$  is the signal from transmitted light in the presence of the magnetic field and  $T(0)$  is that in the absence of the magnetic field. In this section, we also describe how the spectra were obtained.

In Chapter IV, we give plots indicating position of minima in the spectra in a photon energy vs. magnetic field plot. Included in these plots will be calculated lines (fan charts) based on quasi-Ge coupled band  $k \cdot p$   $\rightarrow \rightarrow$  analysis with exciton correction described in Chapter IV.

#### A. Samples

The  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  samples used in this investigation were grown by liquid-phase epitaxy on InP substrates of (100) orientation at Lincoln Laboratory.<sup>1</sup> The InP substrates were Fe-doped to make them semi-insulating. We started our preliminary studies in quaternary sample Q9-6 which yielded only 2-3 minima in the transmission spectrum. The next sample used was Q9-14A with an original

quaternary layer thickness of about  $5\mu\text{m}$ . It turned out that this sample had to be etched a few times to reduce the quaternary thickness until magnetotransmission spectra with four minima were obtained. Finally, a much superior quaternary sample was grown (Q9-18) which yielded 7 to 8 minima in the magnetotransmission spectra. We made the most extensive studies on this sample and on a ternary sample  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  (T9-50) and we shall concentrate on these two samples. Another ternary sample investigated was T9-45A, with somewhat lower electron mobility  $\mu_e$  than T9-50, with no difference in position of minima in the spectra. Table III-1 summarizes some of the characteristics of the two samples studied in detail.

The net impurity concentration  $N_D - N_A$  was measured by the Hall effect, here  $N_D$  and  $N_A$  are the donor and acceptor concentrations, respectively. The quaternary sample has a slight lattice mismatch of  $|\Delta a|/a \approx 1.4 \times 10^{-3}$  where  $\Delta a$  is the difference between the lattice constant of the alloy and the substrate, and  $a$  is the lattice constant of the InP substrate.

#### B. Experimental Setup and Data Acquisition

The experimental setup for magnetoabsorption is depicted schematically in Figure III-1.

In most of the experiments, the optical setup was enclosed in a dry box flushed with dry air to suppress water vapor absorption. A hole was provided in the box directly under the magnet bore to allow the light beam to propagate unobstructed to the sample and back

to the detection side of the optical setup.

### B. 1. The Light Box

This included holders for various light sources. One was for the tungsten lamp which constituted the light source for our experiments. The current through this lamp was set at 9 Amperes using a regulated power supply. Another lampholder was for spectral lamps for the calibration of the grating monochromator. We used the following lamps:

Hg(1.1A); K, Cs, Ne(1.5A).

The light from the lamp was focused on the entrance slit of the grating monochromator by means of a spherical mirror.

### B. 2. Chopper

A 510 Hz, 50% duty-cycle chopper was used to chop the light before entering the monochromator. A square pulse generated by the chopper was used as a reference signal to the PAR 5101 lock-in amplifier.

### B. 3. Grating Monochromator

In most of the experiments the grating monochromator used was a Perkin-Elmer model 99G double-pass grating monochromator. We used Bausch and Lomb gratings with the following specifications, variously: one ruled with 640 lines/mm (blazed for  $1.4\mu\text{m}$ ), two ruled with 600 lines/mm (one blazed for  $1.6\mu\text{m}$  and another for  $1.0\mu\text{m}$ ).

The calibration of the monochromator was performed using the spectral lamps mentioned above. The spectral lines and their wavelengths and energies were identified using the extensive compilation of spectral lines reported in Lincoln Laboratory Report 84G-0012 (1960)<sup>2</sup> for those spectral lamps. It was found out that our calibration was reproducible within 0.1 meV for calibrations done at various times. Also different magnetoabsorption spectra taken on different dates for the same magnet current yielded minima reproducible within 1 meV or less. In the spectral range between 1-1.4 eV with slit width of 0.8 mm using a 600 lines/mm grating resolution of the double pass was 2.5 meV. It was further noted that the resolution scaled linearly with the slit width as large as 1.2 mm and as small as 0.2 mm. Spectra at various slit widths in the above range were taken for the same field values for comparison and to get optimal spectra.

#### B.4. Filters and Polarizers

Filters were used to cutoff higher energy light passing through the monochromator via second or higher order reflection from the grating. Polaroid linear polarizers were used for the Voigt configuration where  $\vec{k}$ , the wave vector of the incident light propagating through the sample is perpendicular to the applied magnetic field  $\vec{H}$ . In this configuration, we chose  $\vec{E} \parallel \vec{H}$  or  $\vec{E} \perp \vec{H}$ ; here  $\vec{E}$  is the oscillatory electric field of the incident light.

For the Faraday configuration ( $\vec{k} \parallel \vec{H}$ ), circular polarizers appropriate to the wavelength range of interest were used. For a

given circular polarizer (made out of a linear polarizer and a quarter-wave plate) the sense of circular polarization of light with respect to the magnetic field could be reversed by reversing the direction of the applied magnetic field. The polarizer could also serve as the filter.

#### B. 5. Directing and Focusing Mirrors

The diverging light emerging out of the monochromator exit slit was folded (by a flat mirror) onto a large long focal length spherical mirror to focus it onto the sample. A 45° adjustable mirror was used to direct this converging light upwards through the bore of the magnet towards the sample. In the Voigt configuration experiments a 4" bore magnet was used. This allowed for a pair of near 45° mirrors on each side of the sample, outside the dewar. The first mirror folded the converging light and allowed it to travel horizontally ( $\vec{k} \perp \vec{H}$ ) through a ZnSe window on the tail of the dewar. The mirrors were arranged to focus the light on the sample. The sample was held vertically in a sample holder attached to the liquid-He cooled cold finger. The light transmitted through the alloy would transmit through the InP substrate unaltered (we used photon energies less than the energy gap of InP which is 1.42 eV). This light then would exit from a second ZnSe window (horizontally) and then would be folded downwards by the 45° mirror in the bore of the magnet. For the Faraday configuration measurements, we used a 2" bore magnet and a different sample holder. The dewar was equipped with a bottom window (sapphire and quartz windows could be used).

The sample holder held two near 45° mirrors to direct the light back down after it has passed through the horizontally held sample (see Figure III-2). The samples in both cases were held in the center of the magnet.

#### B. 6. Collecting Optics and Detector

The diverging light emerging out of the sample and directed down the bore of the magnet was then redirected by means of a second 45° mirror onto another spherical mirror and finally by means of another flat mirror was directed towards the room temperature PbS detector. This light was actually focused by means of a small radius concave mirror onto a very narrow and sharp image right onto the PbS element. The PbS element was biased at 90 volts and the oscillatory photocurrent produced by the chopped light was preamplified.

#### B. 7. Signal Detection and Data Acquisition

The preamplified chopped signal from the detector was then put into a PAR 5101 lock-in amplifier which was referenced with the square pulse from the chopper. The output of the lock-in was both taken to a chart recorder and to channel B of an analog-to digital converter. In each experimental run the magnetic field was held constant and the wavelength of the light emerging out of the monochromator exit slit was swept. This was done by rotating the monochromator drum automatically at a desired speed (1 or 2 minute per revolution). The shaft of a rotary helipot potentiometer was coupled to this drum. The two fixed ends of the potentiometer were connected to a regulated dc voltage source. The angle of the

grating, or equivalently the drum reading, was thus monitored by reading the variable voltage across the variable resistor. The drum reading voltage was then put into the channel A of the A/D converter. The outputs of channel A and B were then punched on paper tape as pairs representing the transmitted signal vs. drum position voltage. These were then taken to the PDP-11/20 computer to process the spectra. The voltage reading on channel A was calibrated in terms of wavelength and photon energy using various spectral lamps described before and reproducibility was excellent ( $\leq 0.1$  meV).

### C. T(H)/T(0) vs. Photon Energy Spectra

The spectra seen on the next few pages were obtained from the data punched on the paper tape using the program Rubin System One (RS1) under DOS-BATCH. The transmitted signal, T(H), taken at the fixed external magnetic field value H, was divided by the zero-field transmitted signal, T(0), point by point. The ratio T(H)/T(0) vs. drum voltage was then converted to the "T(H)/T(0) vs. Photon Energy" spectrum. For this purpose we used our calibration tables (wavelength and photon energy vs. drum voltage) discussed in Section B. 3. In several cases use was made of the smoothing subroutines provided in the RS1 program. Absolute caution was taken to use smoothing very carefully so as not to shift the position of the minima by more than 0.2-0.3 meV. The smoothing helped make a few of the oscillations at higher energies more vivid and this was

always double checked from spectra taken at the same H value at different times and at different slit widths, to eliminate spurious minima.

Figures III-3 through III-9 show some of the spectra for the various fields and polarization, for the two samples Q9-18 and T9-50.

#### D. Point Plots and Fan Charts

The minima appearing in the " $T(H)/T(0)$  vs. Photon Energy" spectra were then tabulated against the H-values for each polarization configuration for each sample as described in Chapter IV. The photon energies of these minima were plotted vs. H. These point plots, and the associated fan charts which are the result of the quasi-Ge coupled band analysis with exciton corrections, will be explained in Chapter IV.

TABLE III-1 Some characteristics of the two epitaxial  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  samples, grown on InP substrates, which were used for the interband magneto-optical measurements reported in this thesis.

Sample	x	y	$\frac{\Delta a}{a}$	$N_D - N_A$ ( $\text{cm}^{-3}$ )	$\mu_e(77\text{K})$ ( $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ )	Epilayer Dimensions		Orientation		* $E_g$ (eV)
						Thickness ( $\mu\text{m}$ )	Edges (mm x mm)	Thickness	Edges	
Q9-18	0.25	0.52	$1.4 \times 10^{-3}$	$2.7 \times 10^{15}$	11,000	1.8	5.5x8	along [100]	along [100] directions	1.065
T9-50	0.47	1.0	$\lesssim 0.6 \times 10^{-3}$ **	$1.4 \times 10^{16}$	24,000	4.4	3x8	along [100]	along [110] directions	0.813

\* Obtained from our interband magnetoabsorption experiments near liquid-He temperature.

\*\* This is the limit of resolution of the x-ray apparatus.

FIGURE III-1 Schematic diagram of the experimental setup for the magnetotransmission experiments. In this Figure the sample is setup for the Voigt configuration where the wave vector of light  $\vec{k}$  through the sample is normal to the direction of applied magnetic field  $\vec{H}$ . The sample geometry for Faraday configuration where  $\vec{k}||\vec{H}$  is shown in Figure III-2.

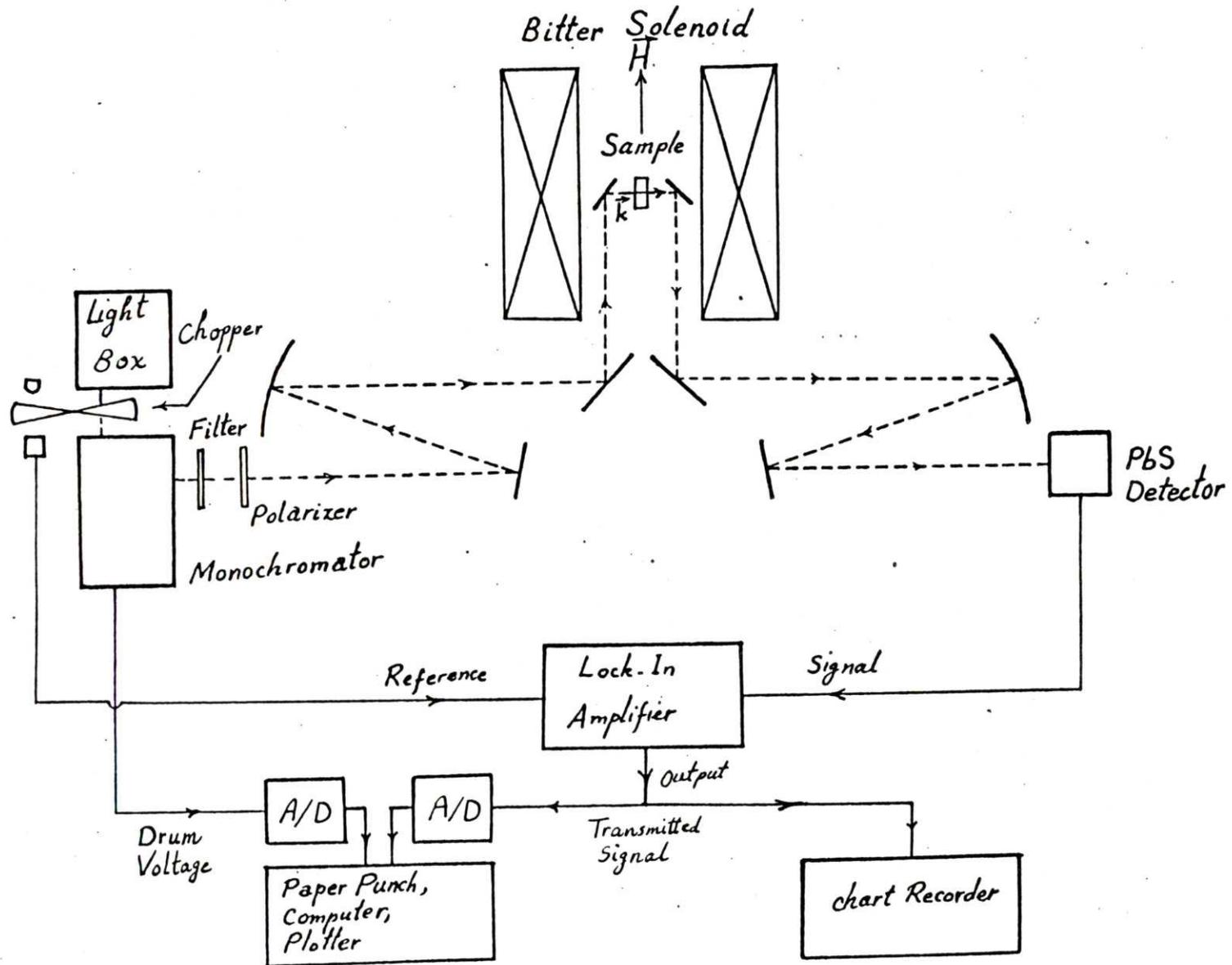


FIGURE III-2 The sample geometry for the Faraday configuration where the light propagation vector  $\vec{k}$  through the sample is parallel to the direction of applied magnetic field,  $\vec{H}$ . In this Figure S represents the sample and M represents two flat mirrors, at nearly  $45^\circ$  with respect to  $\vec{H}$ .

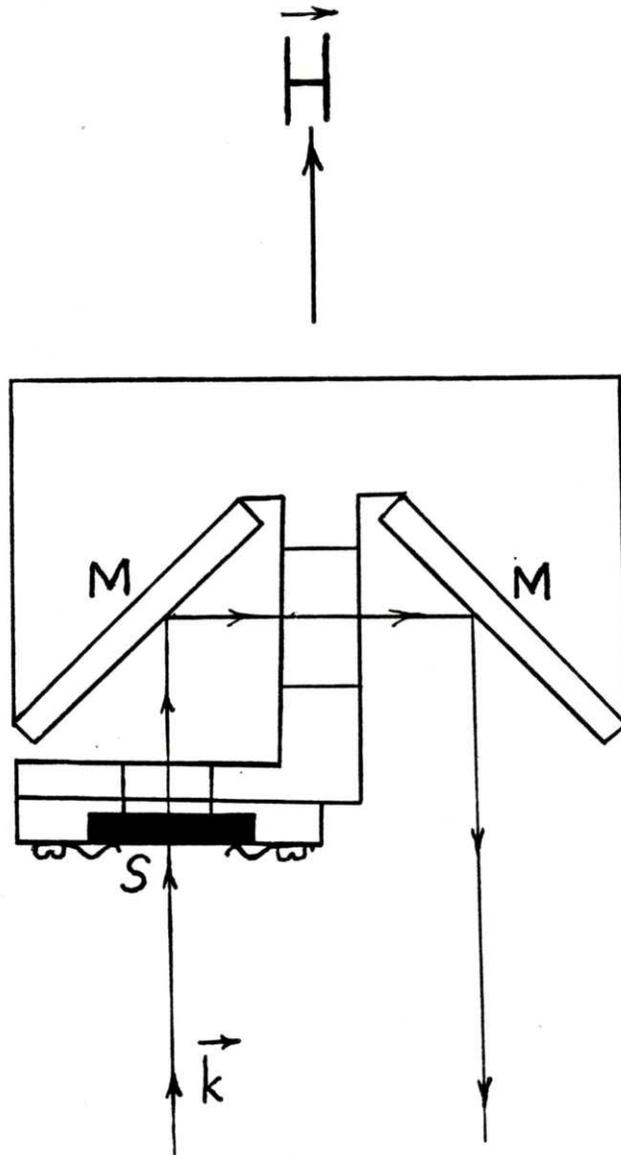


FIGURE III-3 Voigt configuration  $\vec{E} \parallel \vec{H}$  interband magnetotransmission spectrum for Q9-18, taken at near liquid-He temperature, at  $H=130.5$  kOe. Bars at the bottom of the figure indicate the calculated positions and their heights are proportional to the square of matrix elements for transition from light (+) and heavy (-) hole magnetic subbands to the conduction magnetic subbands (see Chapter IV).

To represent relative intensities, the light-hole bars should be shortened by a factor of  $(m_+/m_-)^{1/2} \approx 2.4$  to approximately account for the difference in the density of states.

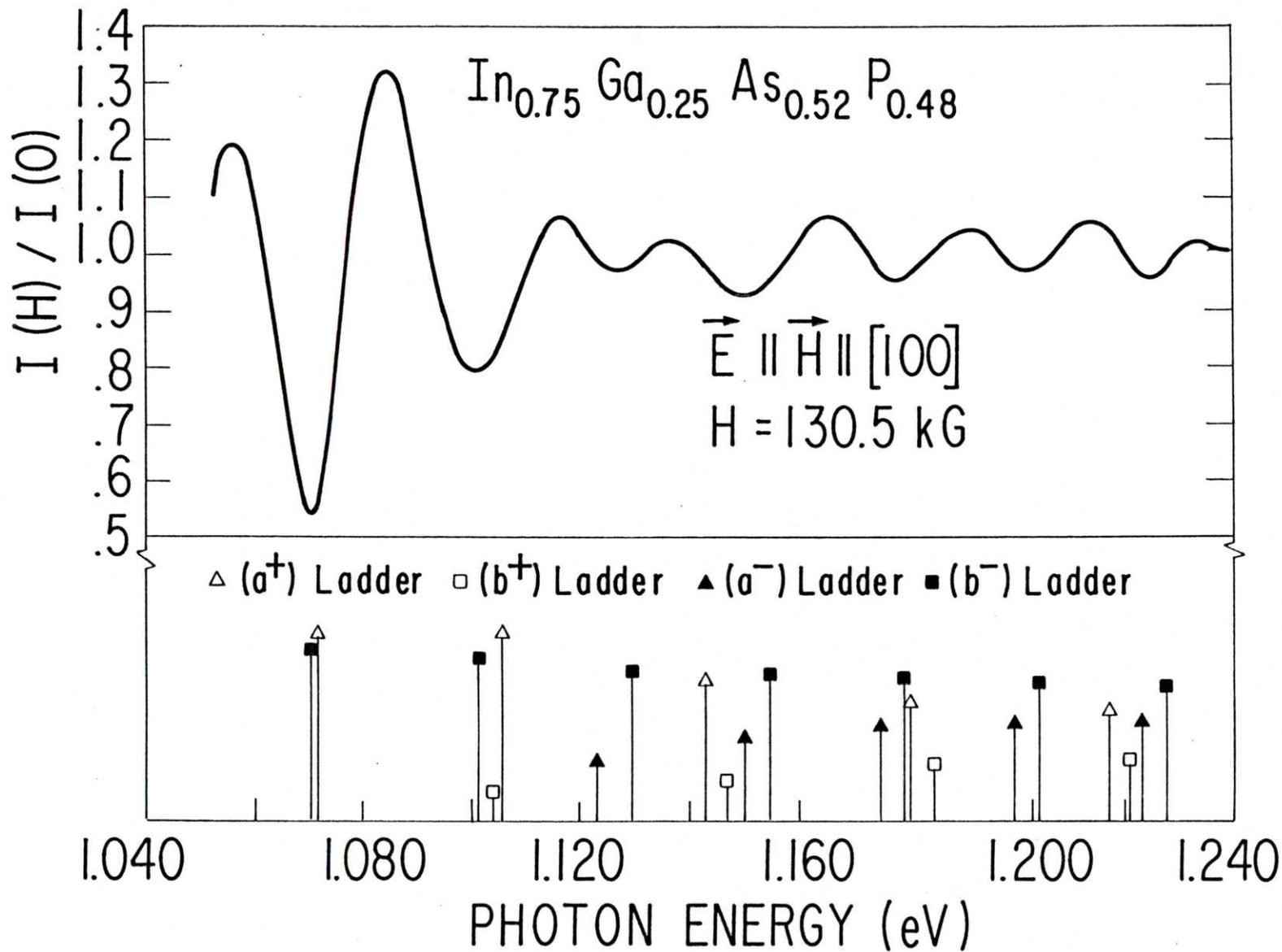


FIGURE III-4 Faraday configuration magnetotransmission spectrum for right circularly polarized light (RCP) taken at 143.9 kOe in the quaternary sample Q9-18 in contact with a liquid-He cold finger.

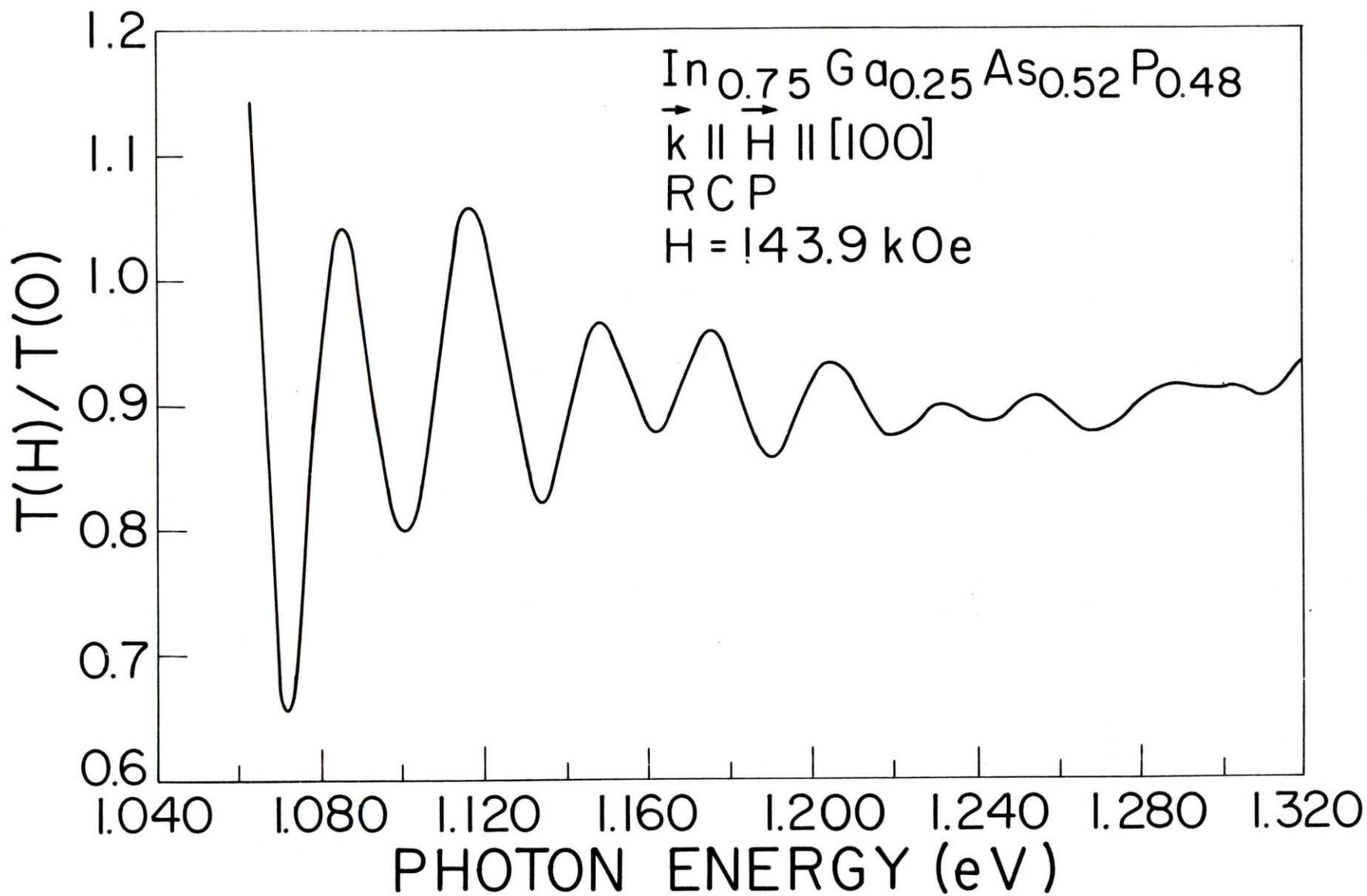


FIGURE III-5 Faraday configuration magnetotransmission spectrum for left circularly polarized light (LCP) taken at 143.9 kOe in the quaternary sample Q9-18 in contact with a liquid-He cold finger.

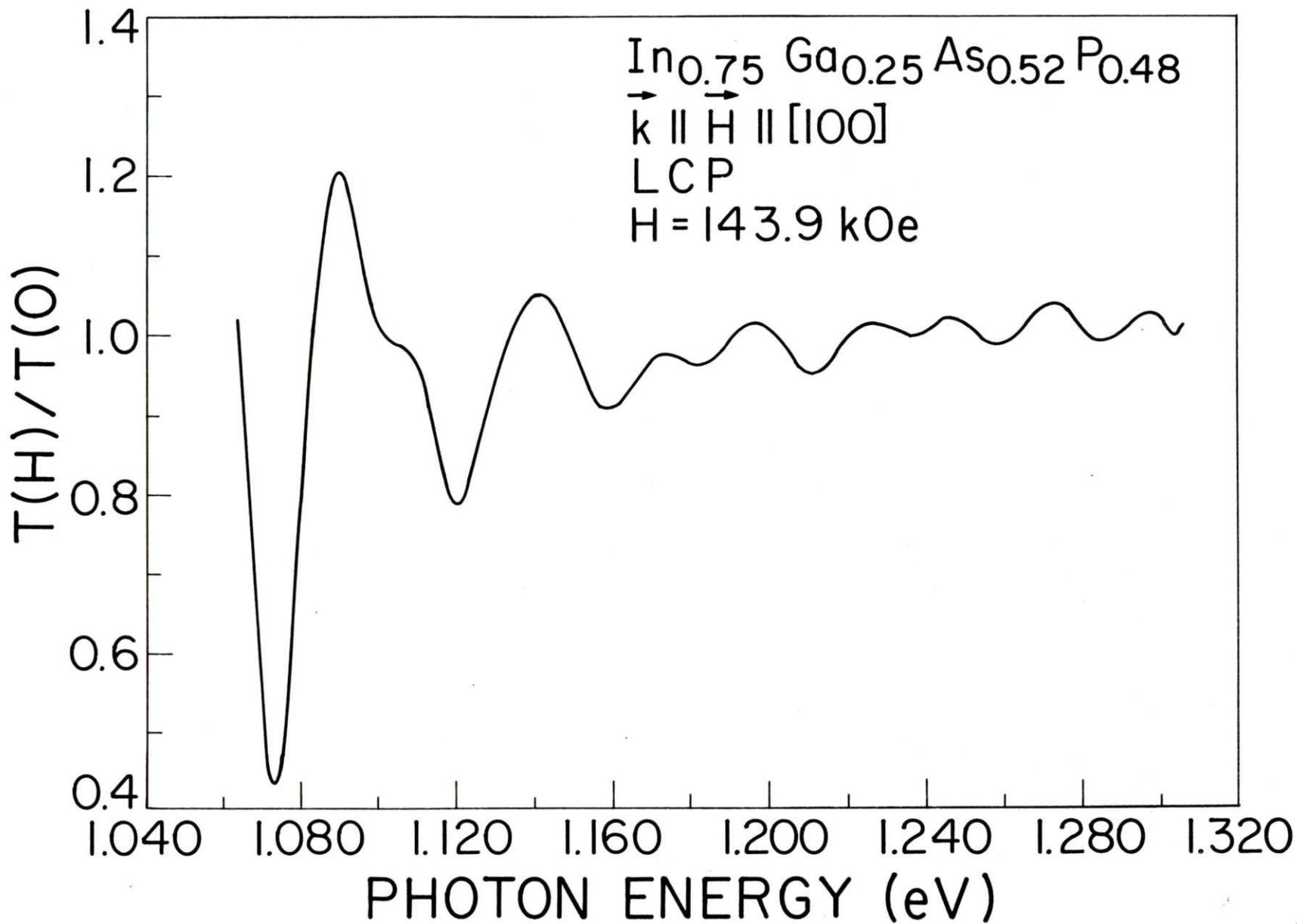


FIGURE III-6 Faraday configuration  $\vec{k} \parallel \vec{H}$  magnetotransmission spectra for left and right circularly polarized light (LCP and RCP) taken at 137.2 kOe for in the sample T9-50 in contact with a liquid He cold finger.

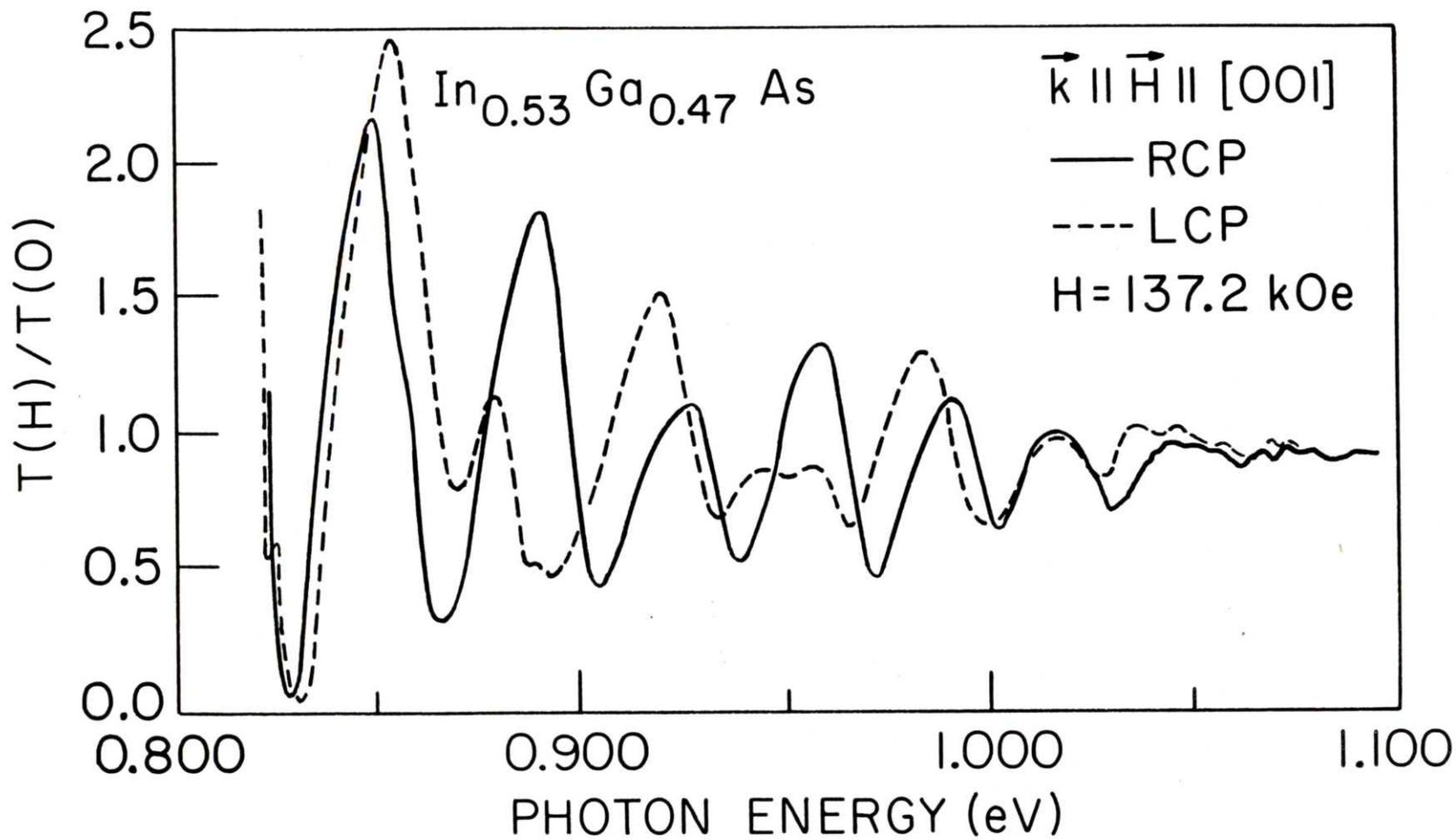


FIGURE III-7 Faraday configuration ( $\vec{k} \parallel \vec{H}$ ) magnetotransmission spectra for left and right circularly polarized light (LCP and RCP), for the sample T9-50 in contact with a liquid-He cold finger, with  $H=137.2$  kOe. The intensity bars beneath each spectrum indicate calculated energy positions, and their heights are proportional to the square of matrix elements for optical transitions from light (+) and heavy (-) hole to conduction electron Landau levels. Light hole intensity bars are reduced by a factor of  $(m_-/m_+)^{1/2}$  to reflect the difference between light and heavy hole densities of state approximately. (See Chapter IV.)

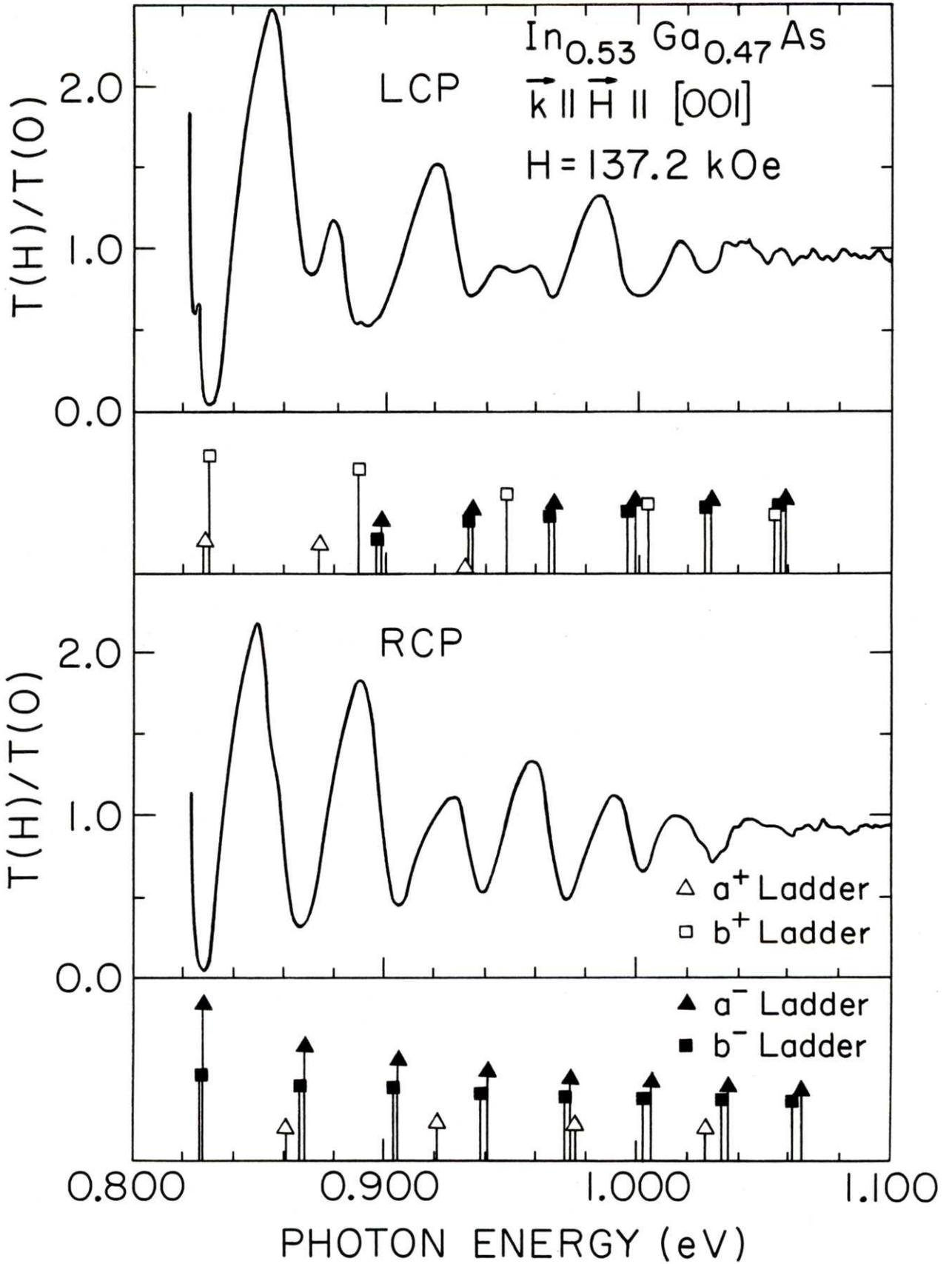


FIGURE III-8 Magnetotransmission spectrum in the Voigt configuration for light polarized with  $\vec{E} \parallel \vec{H}$  taken at  $H=126.9$  kOe in the sample T9-50 in contact with a liquid He cold finger. For a description of the bars under the spectrum see Figure III-7 caption.

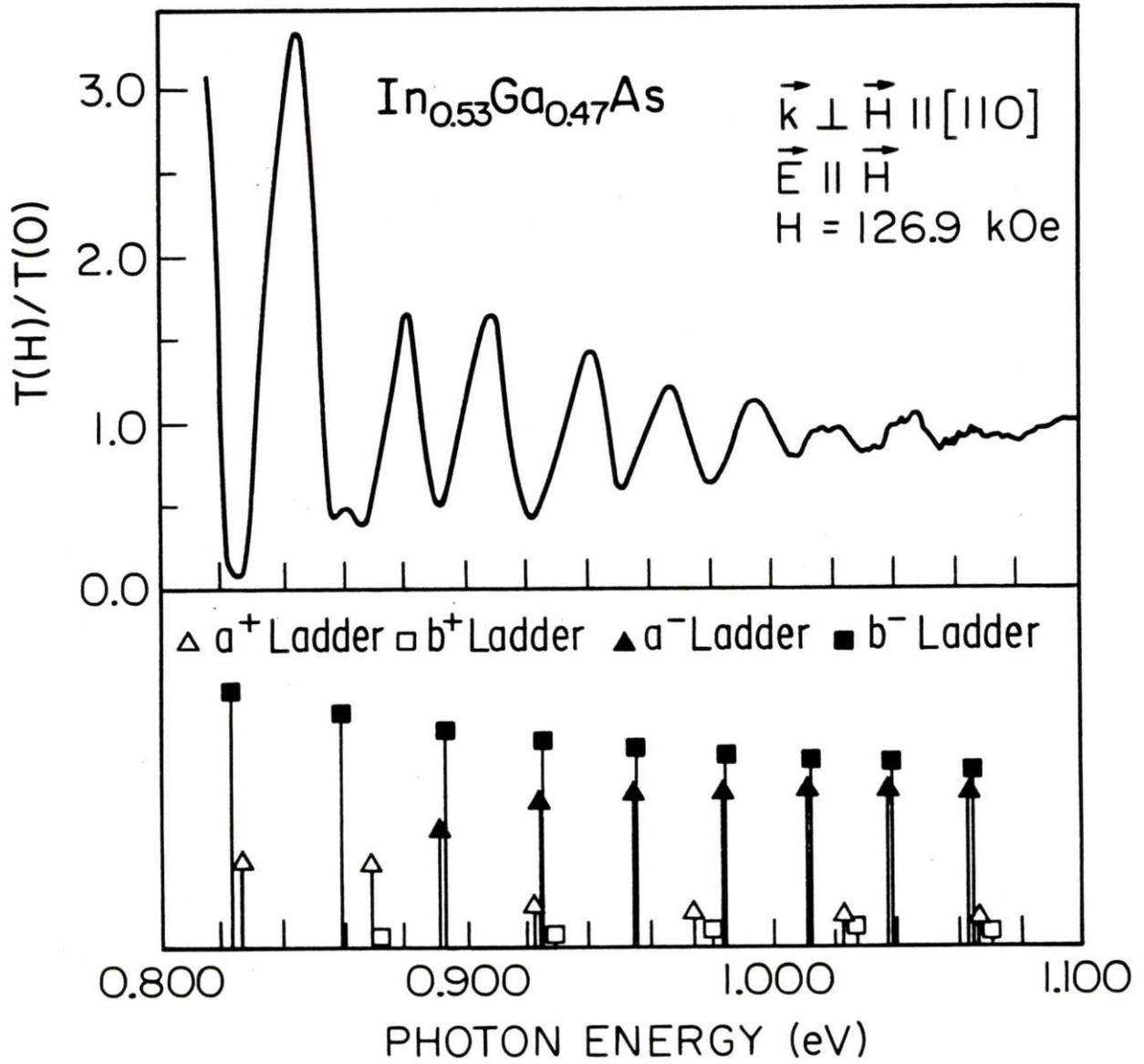
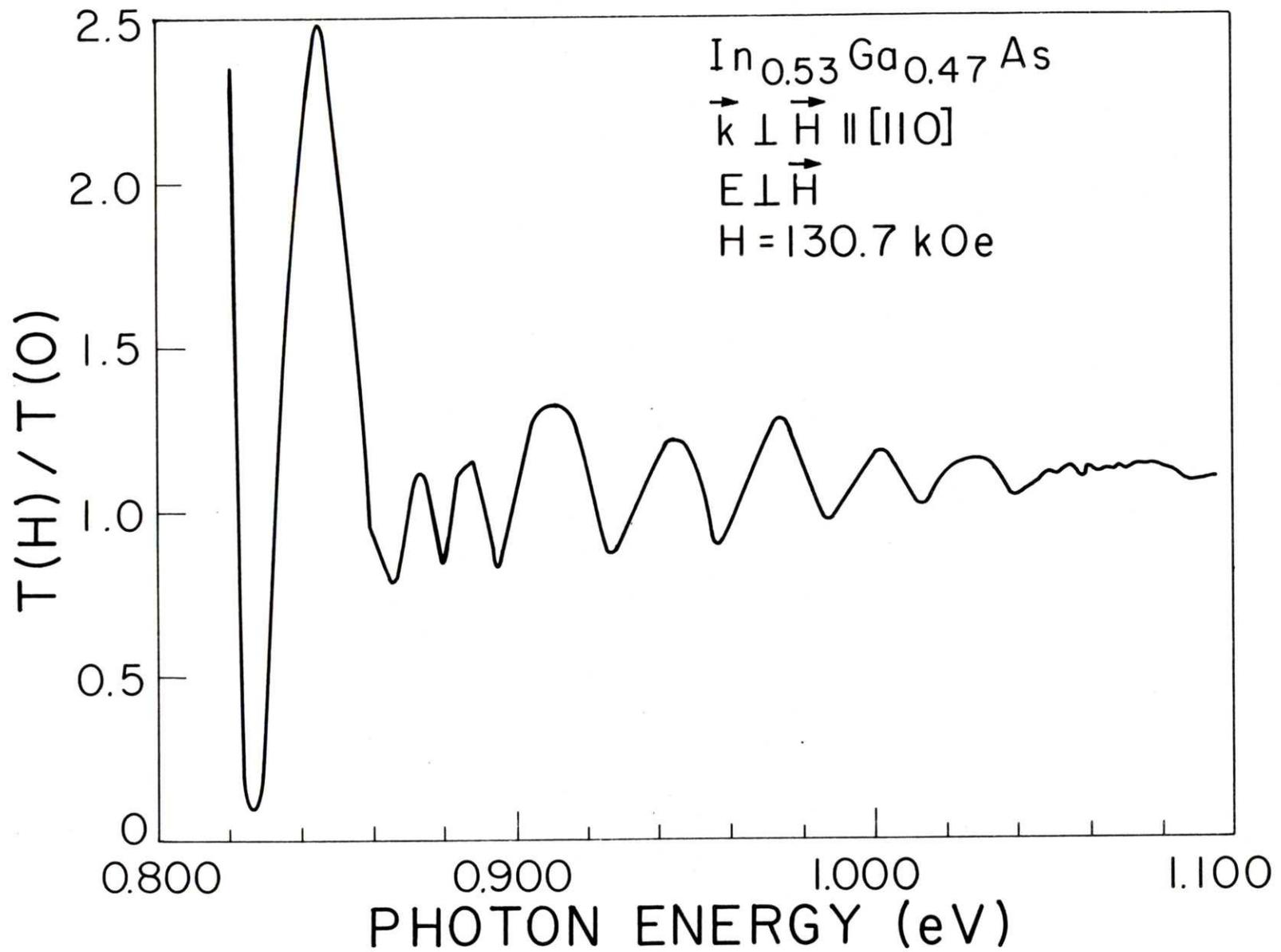


FIGURE III-9 Magnetotransmission spectrum in the Voigt configuration for light polarized with  $\vec{E} \perp \vec{H}$  taken for the sample T9-50 in contact with a liquid-He cooled cold finger at  $H=130.7$  kOe.



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## CHAPTER IV

### ANALYSIS AND RESULTS

The quasi-Ge coupled band theory reviewed in Chapter II has been used to determine the  $\vec{k}\cdot\vec{p}$  band parameters from our interband magnetoabsorption spectra in the ternary and the quaternary samples which was presented in Chapter III.

In this chapter we give the steps involved in applying this model to our experimental spectra. Next, we present the band parameters which we have obtained for our samples together with the fan charts calculated from the quasi-Ge model. At the end of this chapter a discussion of the results will be presented.

#### A. Analysis of the Spectra in Terms of the Quasi-Ge Model

##### A. 1. An Outline

In this section we present an outline of the steps involved in the analysis of the magnetoabsorption spectra, "T(H)/T(0) vs. Photon Energy" in the context of the quasi-Ge model reviewed in Chapter II. These are the steps involved:

##### Step I -- Examination of the T(H)/T(0) Spectra

The minima are assumed to emanate from the interband optical transitions from the valence band magnetic sub-bands to the conduction band magnetic sub-bands (Landau levels). The details will be given in Section A. 2.

## Step II -- Identification of the Minima

Attempts are made to identify each minimum with one or more such transition mentioned above, if at all possible.

### Step IIa -- Experimental Identification: Point Plots

For a given minimum in the spectrum the experiment gives us the following information (a) the photon energy  $E$ , (b) the magnetic field value  $H$ , (c) the spherical coordinate angles  $(\theta, \phi)$  made by  $H$  with respect to the cubic axes of the crystal, and (d) the polarization state of light, i.e. ( $\sigma_R, \sigma_L$  in the Faraday configuration,  $\vec{E} \parallel \vec{H}$ ,  $\vec{E} \perp \vec{H}$  in the Voigt configuration), and (e) relative strength and width of the minimum (some minima are stronger, some weaker, some are too close to be distinguishable, and some even appear as inflection points or shoulders). At this step, for each  $H$ -orientation (c) and light polarization configuration (d) we make a separate plot of  $E(\text{meV})$  vs.  $H(\text{kOe})$  for all of the minima in the spectra, with the same (c) and (d) conditions. We refer to these as point plots.

### Step IIb -- Assignment of Transition Labels to the Minima

Now given these five attributes (a)-(e) for a minimum, we should in general be able to use the quasi-Ge model (with the correct set of band parameters) to gain the following missing information about that minimum: which interband magneto-optical transition (transitions) are responsible (or most likely responsible) for this minimum? If the correct set of band parameters is used one is able to answer the above with the following quantities or attributes: (f) the initial state in

the valence band, i.e. whether it is  $a^-$ ,  $b^-$ ,  $a^+$  or  $b^+$ , (g) the Landau quantum number of the initial state "n". Now with this specification, the final state in the conduction band (h) is automatically specified subject to the selection rule for the magneto-optical transition in the specific polarization state(d). By conduction band specification (h) we mean whether the final state is  $a^c(n')$  or  $b^c(n')$  and what value  $n'$  has. Finally, a correct set of quasi-Ge parameters ought to give at least a qualitatively good agreement between the calculated and the observed strengths of transitions.

To carry out Step IIb one therefore needs a set of initial parameters, which are reasonably close to the actual values, to start the analysis. Therefore, before Step IIb can be taken we need to go to Step III:

Step III -- Initial set of Band Parameters for the Start of the Analysis:  
Values for the Quasi-Ge Model

This is an important step; the initial set of values for the quasi-Ge band parameters, i.e.,  $E_g$ ,  $E_p$ ,  $\Delta$ ,  $\gamma_1$ ,  $\gamma_2$ ,  $\gamma_3$ ,  $\kappa$ ,  $F$ ,  $q$ , and  $N_1$ , has to be selected judiciously and has to be as much based on physical consideration as possible.

Step IV -- Exciton Corrections

The observed experimental values for the energy of the minima are affected (in fact reduced) by the excitonic binding energies (see Section A.3. for details). Therefore, if we are to apply the quasi-Ge model to calculate energies for the interband

magneto-optical transitions (in order to make contact with the experimentally observed values of the energies), we have to subtract an appropriate amount (depending upon  $n'$  and  $H$ ) according to the prescriptions of Section A.3. This can be done right after the transition energy for a particular transition and  $H$  value is calculated in the computer program.

Step V -- Relative Intensities of Transitions: To Determine Which Allowed Transitions are too Weak to be Included in the Analysis

Suppose one has the correct band parameters for the given sample. For a given polarization condition ( $d$ ) there are a vast number of allowed interband magneto-optical transitions from the valence  $\{a^-(n), b^-(n), a^+(n), b^+(n)\}$  magnetic sub-bands to the conduction  $\{a^c(n), b^c(n)\}$  magnetic sub-bands. It turns out that a good number of these transitions are too weak relative to the rest and hence experimentally not observable. Therefore, it is desirable (and in fact necessary) to exclude these transitions (although allowed) from the analysis. This does not mean that all of the weak transitions are eliminated. In fact, the relative strengths of the minima vary from one minimum to another in a given spectrum (usually diminishes as  $E$  is increased) and from one polarization to another (see Figures III-3 through III-9). There are some weak transitions which are still observable. However, it turns out that transitions from the  $a^+$  light-hole series occur mainly for RCP while those originating from  $b^+$  light-hole series occur mainly for LCP.

### Step VI -- Fan Charts Using Initial Band Parameters

Having decided, on the basis of Step V, which of the allowed transitions ought to be included in the analysis, we are then ready to generate fan charts (see Figures in this chapter). A fan chart is a family of lines generated from calculated transition energies as a function of  $H$  using a set of band parameters. Each line represents a particular transition from the set  $\{a^-(n), b^-(n), a^+(n), b^+(n)\}$  to the set  $\{a^c(n), b^c(n)\}$  allowed by the selection rule for optical transitions in the particular polarization configuration, (d) and  $H$ -orientation (c). If the initial parameters are chosen judiciously (i.e., are chosen close to the correct values) then in general each calculated line, with a few exceptions, will pass reasonably close by (in some cases very close by) a family of points in the "point plot" (the family representing a particular minimum as it evolves with increasing  $H$ ). For some of the minima more than one calculated line will pass close by, indicating that those minima correspond to a set of close lying transitions. It turns out that it is generally possible to choose a reasonable initial set of band parameters to make correct identification of the minima (points on the point plot). The identification completes Step IIb.

### Step VII -- Data Files

With the above initial identification of the points on the point plots, we now can generate data files for a given sample and a given  $H$  orientation. Each point on the data file includes five numbers:  $\{IP, IT_1, IT_2, H, E\}$  where  $IP$  is the polarization state of

light, IT is the label for the identification of transition (see Step VI), where up to two transitions can be accommodated, H is the magnetic field value and E, the transition energy given by the experimental spectra. In this manner, we include all or most of the points on the "point plot". These data files are then stored to be used in a minimization routine.

#### Step VIII -- Minimization Routine: Search for Optimum Band Parameters

The data files constructed according to Step VI, are now used as inputs for a minimization routine. The minimization routine asks for input of the data files, the direction of H with respect to cubic axes of the crystal, and a set of values for the quasi-Ge band parameters ( $E_g$ ,  $E_p$ ,  $\Delta$ ,  $\gamma_1$ ,  $\gamma_2$ ,  $\gamma_3$ ,  $\kappa$ , F, q,  $N_1$ ). It also asks for identification of those parameters we may wish to vary; it also provides for constraint equations that we may wish to impose on these parameters, for instant to fix  $m_c$  or  $m_-$ . For each point in the data file (see Step VII) the program then calculates the transition energy in the quasi-Ge model and compares this with the given experimental energy. The program thus calculates the deviation of these two energies for each point and determines the root mean square deviation:

$$\Delta = \left\{ \frac{1}{N} \sum_{i=1}^N [E_i(H) - E_i]^2 \right\}^{1/2} \quad (4-1)$$

where  $E_i(H)$  is the calculated transition energy of the data point  $i$  and  $E_i$  is the stored energy value of this data point, and  $N$  is the number of such points.

The correct band parameters are expected to be obtained by an iterative method described by Reine<sup>1,2</sup> and incorporated by Weiler<sup>3,4</sup> in the computer program. In each iteration a new set of band parameters are calculated based upon the old ones, so as to minimize  $\Delta$ . Details will be given in Section A.4.

This minimization routine is used until a set of band parameters are found which minimize  $\Delta$ , subject to certain constraints on the band parameters which are based upon physical consideration. Otherwise, one cannot even hope for convergence. This is very important and makes the task in Step III very crucial. We will discuss these points (initial band parameters, necessary constraints, and the performance of the minimization routine) later on in this Chapter in some detail.

#### Step IX -- Checking Band Parameters Obtained in "Step VIII"

The set of band parameters which minimize the rms deviation mentioned in Step VIII are presumably those which most closely represent the true band structure of the semiconductor. This has to be tested; some of the relevant questions are:

- 1) How well do these parameters represent the bands from physical point of view and how well do they predict other measurements, by other methods, of these parameters directly or indirectly?

- 2) How well do these parameters explain the magneto-optical data, i.e., how closely do the new fan charts represent the data points on the point plots, and how do the newly calculated relative intensities compare with the  $T(H)/T(0)$  spectra?
- 3) Do these new parameters give the same initial identifications deduced in Steps VI and IIb?
- 4) What range of values can these parameters accept and still give good fits with the experimental data, while remaining physically meaningful?
- 5) What can be learned from interband magneto-optical measurements on these samples?

#### A. 2. Details Involved in Step 1

The starting point for the analysis of the magneto-absorption data is the examination of the " $T(H)/T(0)$  vs. Photon Energy" spectra where  $T(H)$  is the signal from the infrared radiation transmitted through the sample in the presence of magnetic field and  $T(0)$  is that for  $H=0$ . The observed minima in these spectra are assumed to be due to interband optical transitions from the valence to the conduction band magnetic band magnetic sub-bands (Landau levels). More explicitly, these transitions are from the Landau levels of the  $\Gamma_8^V$  valence bands  $|a^-(n)\rangle$ ,  $|b^-(n)\rangle$ ,  $|a^+(n)\rangle$ , and  $|b^+(n)\rangle$ , to the magnetic sub-band (Landau levels) of  $\Gamma_6^C$  conduction band, i.e.  $|a^C(n')\rangle$ , and  $|b^C(n')\rangle$  (see Ch.II). This is a very

important assumption upon which the whole analysis hinges. The justification for this comes from (i) the fact that all of the minima occur at energies higher than the band gap of the material, (ii) the shape of the spectra for a given polarization geometry remains essentially the same as one examines the spectra for different H values and the positions of minima shift towards higher photon energy and their distances increase with increasing H, and (iii) the assumption stated above have worked very well in explaining magneto-absorption and magnetoreflexion spectra of InAs, GaAs, InP and many other semiconductors. (See for example review articles by Lax and Mavroides<sup>5</sup> and Aggarwal.<sup>6</sup>) It is also possible to have transitions from the spin-orbit split-off ( $\Gamma_7^V$ ) band Landau levels to the conduction band ( $\Gamma_6^C$ ) Landau levels such as observed by Groves and coworkers in Ge<sup>7</sup> and III-V compounds,<sup>3</sup> by Reine<sup>1,2</sup> and coworkers<sup>7,10</sup> in GaSb and GaAs, and by Aggarwal,<sup>11</sup> in Ge, among others. However, these observations were possible only in modulated magnetoreflexance and not magnetoabsorption. In our case the magneto-optical transitions from the split-off to the conduction band would be expected to occur in the tail region of the spectra where the fundamental edge absorption is high and signal to noise ratio is too low to observe such transitions by the magnetoabsorption method.

One final note concerning the spectra. Because of the linewidths involved and the richness of the structure, some close lying transitions would appear as one and there could be relatively small pulling and pushing of peaks. Also, some weaker transitions

(usually light hole transitions) are seen as inflection points or are buried in the wings of a strong transition, as mentioned earlier. This means that there is inherent approximation as far as the energy positions of transitions are concerned. Hence, good quality crystals with good homogeneity and high mobility and low temperatures are a necessary condition for obtaining finely resolved spectra. Modulation techniques (e.g. the magnetoelectroreflectance experiments of Refs. 7 and 8 which were performed at room temperature) will further enhance the fine resolution of the spectra.<sup>1,2,6</sup>

### A. 3. Exciton Corrections

It is known that in many semiconductors, such as InP<sup>12</sup> and GaAs<sup>13,14</sup> which are among the constituents of the quaternary system under consideration, the electron-hole pair, which is created by the optical excitation, can bind together to create "free excitons" in much the same way as an electron-positron pair can bind together to form a bound positronium "atom". In case of semiconductors this e-h binding lowers the transition energy by a small amount (typically a few meV). This energy  $E_B$  is the so-called binding energy, ( $E_B > 0$ ). The problem of exciton in a magnetic field is an interesting, but complicated problem.<sup>14-21</sup> In the case of our experiments, we are not concerned with the fine structure of excitations, since our linewidths are too large for that. Thus we include the effect of excitonic binding energy using a simpler method used by Vrehen.<sup>14</sup> According to this method, the transition energies

calculated in the quasi-Ge model are reduced by subtracting the approximate binding energy  $\Delta E(n,H)$ . Here  $n$  refers to the Landau quantum number of the final state (conduction band) and  $H$  is the magnetic field value. In the case of  $n=0$ , Vrehan uses

$$\Delta E(0,H) = E_B(\gamma) \cdot R \quad (4-2)$$

and for higher  $n$ 's

$$\Delta E(n,H) = E_B\left(\frac{\gamma}{2n+1}\right) \cdot R \quad (4-3)$$

where  $\gamma$  is the reduced magnetic field,  $R$  is an effective Rydberg energy, and  $E_B(\gamma)$  is the binding energy (defined  $>0$ ) of a hydrogen-like atom in a magnetic field (reduced field) in units of  $R$ . Here

$$R \equiv R_0(\mu/m)/\kappa_e^2 \quad (4-4)$$

and

$$\gamma \equiv \mu_B H(m/\mu)/R \quad (4-5)$$

where  $\kappa_e$  is the static dielectric constant,  $R_0$  is the atomic Rydberg constant,  $\mu_B$  the Bohr magneton,  $m$  the free electron mass, and

$$\mu^{-1} = m_c^{-1} + m_{\pm}^{-1} \quad (4-6)$$

is the reduced mass for transition from light (+) and heavy (-) holes to the conduction band.

We have included the effect of nonparabolicity in an approximate manner by using a field-dependent effective mass

$$\mu(n,H) \approx \mu [1 + 4(2n+1)\mu_B H(m/\mu)/E_g]^{1/2} \quad (4-7)$$

(it turns out that this results in a very small correction of  $\leq 1$  meV for the highest  $n$  and  $H$ ).

For  $E_B(\gamma)$  we have used unpublished numerical results of Larsen based on his paper.<sup>19</sup> See Table IV-1 for  $E_B(\gamma)$  vs.  $\gamma$ . These values of  $E_B$  are for the 1S ground state, and are in agreement with those obtained by Praddaude.<sup>20</sup> The high  $\gamma$  values are also in very good agreement with Altarelli and Lipari (for  $\gamma > 5$ )<sup>17</sup> and Johnson and Dickey<sup>21</sup> who find  $E_B(\gamma) \approx 1.6\gamma^{1/3}$  for large  $\gamma$ .

The method of Vrethen, namely using Eq.(4-3) for  $n > 0$ , agrees well with Table V of Ref. 17 which gives the binding energies for  $\gamma \geq 5$  for  $n=0, 1, \text{ and } 2$ , and  $\ell=0$  series of hydrogenic exciton.

#### A. 4. Minimization Routine

We have used for our minimization routine, the method described by Reine<sup>1</sup> and adopted by Weiler.<sup>3</sup> This approach is an iterative one based on a generalized method of least squares.

Let  $\vec{x} = (x_1, \dots, x_j, \dots, x_M)$  be the set of  $M$  band parameter used in the quasi-Ge model analysis (e.g.,  $x_1 = E_g$ ,  $x_2 = E_p$ ,  $x_3 = \gamma_1$ , etc.). Furthermore, suppose there is a set of values for these parameters,

say  $\vec{x}^0 = (x_1^0, x_2^0, \dots, x_M^0)$ , which represents the  $\Gamma_6^C$ ,  $\Gamma_8^V$ , and  $\Gamma_7^V$  bands of the semiconductor under study most closely. Let  $E(H_i; \vec{x}^0)$  be the calculated transition energy corresponding to the  $i$ th point in the data file (Steps II and VII) with the magnetic field  $H_i$ . Then these energies most closely represent the experimental transition energies. Now suppose we start out with an approximate set of band parameters  $\vec{x}$  to start our analysis, then the corresponding calculated transition energies will be  $E(H_i; \vec{x})$ ; and the rms deviation would be

$$\Delta(\vec{x}) = \left\{ \frac{1}{N} \sum_{i=1}^N [E(H_i; \vec{x}) - E(H_i; \vec{x}^0)]^2 \right\}^{1/2} \quad (4-8)$$

Let  $D(\vec{x}) = N[\Delta(\vec{x})]^2$ . Values of  $\vec{x}$  which minimize  $D(\vec{x})$  will also minimize  $\Delta(\vec{x})$ . The derivatives of  $D(\vec{x})$  with respect to the band parameters  $x_m$  are

$$\frac{\partial D(\vec{x})}{\partial x_m} = \frac{2}{N} \left[ \sum_{i=1}^N F_m(H_i; \vec{x}) [E(H_i; \vec{x}) - E(H_i; \vec{x}^0)] \right] \quad (4-9)$$

where

$$F_m(H_i; \vec{x}) \equiv \frac{\partial E(H_i; \vec{x})}{\partial x_m} \quad m=1, \dots, M \quad (4-10)$$

Now according to the mean value theorem of calculus, there exists a number  $\lambda$ ,  $0 \leq \lambda \leq 1$ , such that

$$E(H_i; \vec{x}) - E(H_i; \vec{x}^0) = \sum_{n=1}^M F_n(H_i; \vec{x}^C) (\vec{x}_n - \vec{x}_n^0) \quad (4-11)$$

where  $\vec{x}^C = \lambda \vec{x} + (1-\lambda) \vec{x}^0$

(Note that  $\lambda$  and therefore  $\vec{x}^C$  is not necessarily unique unless  $\vec{x}$  is chosen close enough to  $\vec{x}^0$ . This makes the choice of initial approximate values  $\vec{x}$  crucial.) Equation (4-9) becomes:

$$\begin{aligned} \frac{N}{2} \frac{\partial D(\vec{x})}{\partial x_m} &= \sum_{i=1}^N F_m(H_i; x) [E(H_i; x) - E(H_i; x^0)] \\ &= \sum_{i=1}^N F_m(H_i; \vec{x}) \sum_{n=1}^M F_n(H_i; \vec{x}^C) (x_n - x_n^0) \end{aligned} \quad (4-12)$$

This gives

$$\sum_{n=1}^M A_{mn}^C \xi_n = B_m \quad m=1, \dots, M \quad (4-13)$$

where

$$\xi_n \equiv x_n - x_n^0 \quad (4-13a)$$

$$B_m \equiv \sum_{i=1}^N F_m(H_i; \vec{x}) [E(H_i; \vec{x}) - E(H_i; \vec{x}^0)] \quad (4-13b)$$

$$A_{mn}^C \equiv \sum F_m(H_i; \vec{x}) F_n(H_i; \vec{x}^C) \quad (4-13c)$$

The term  $B_m$  is determined by the guess  $\vec{x}$  and the experimental points  $E(H_i; \vec{x})$ , therefore, it can be regarded as the external forcing term in the linear Eq.(4-13). The error  $\xi_n$  are the unknowns since  $x_n^0$  are unknown. The matrix  $A_{mn}^C$  is also unknown since  $\vec{x}^C$  is unknown. However, Eq.(4-13) lends itself to an iterative solution (convergence not guaranteed, unless  $\vec{x}$  is "close enough" to  $\vec{x}^0$ ):

- (1) Chose  $\vec{x}$ , i.e. a set of values for the band parameters, close to the unknown true values  $\vec{x}^0$ .
- (2) Calculate  $E(H_i; \vec{x})$  and  $F(H_i; \vec{x})$ , using quasi-Ge model. For F see Appendix B of Ref. 3.
- (3) For  $E(H_i; \vec{x}^0)$  use the experimental transition energies, since  $E(H_i; \vec{x}^0)$  values are supposed to give the best estimates for the latter.
- (4) Calculate  $\Delta(\vec{x})$ , the rms derivation using Eq.(4-8).
- (5) Use (1) and (2) to calculate  $B_m$ .
- (6) Approximate  $F_n(H_i; \vec{x}^c)$  by  $F_n(H_i; \vec{x})$ .
- (7) Calculate  $A_{mn}^c$  using (2) and (5).
- (8) Solve Eq.(4-13) to obtain approximate errors  $\xi_n$ .
- (9) Replace  $\vec{x}$  by  $\vec{x} - \vec{\xi}$ . These are new guesses for the band parameters.
- (10) Use the new  $\vec{x}$ 's and go to (2) and repeat steps (2) through (9) until  $\Delta(\vec{x})$  shows convergence to a stationary value.

This procedure is the essence of the minimization routine. It can accommodate constraint equations among  $x_m$ 's by the method of Lagrange multipliers. If the process is convergent then after each step,  $\vec{x}$  (and therefore  $\vec{x}^c$ ) gets closer to  $\vec{x}^0$  and  $B_m$  gets smaller and step (6) becomes more and more justifiable, i.e.  $A_{mn}^c$  gets progressively closer to  $A_{mn}$  and  $(\partial D / \partial x_m)$  gets progressively smaller. We should note that step (3) is inherently an approximation which the analysis cannot do anything about, because of experimental uncertainties.

The details of the computer program which incorporates this minimization technique within the context of the quasi-Ge model are given in Ref. 3 (see especially Appendix B and C, thereof). In step (2) above, the calculated  $E(H_j; \vec{x})$  which we have used includes the exciton binding energy corrections which we described in Section A.3. However, in calculating the derivatives  $F_m(H_j; \vec{x})$  the exciton corrections are ignored in  $E(H_j; \vec{x})$  since these derivatives are not nearly as sensitive to these corrections as  $E(H_j; \vec{x})$  is.

#### B. Determination of the Band Parameters

As it was mentioned in Section A, to obtain the band parameters in the quasi-Ge model, we need to start with a set of band parameter values which are reasonably close to the "true" values. (Section A.1, Step III.) These initial parameters are then used in computer programs to generate fan charts, identify transitions, estimate intensities of the transitions, generate data files, and then use the minimization routine to improve the fit. This is like a boot-strap operation. The questions that we shall address in this Section are: (1) what parameters can we determine directly from the spectra (or point plots) right at the onset without the full use of the complicated computer analysis? (2) Which transition can we identify right at the outset? (3) Which of the quasi-Ge parameters are too small to affect our analysis (and therefore not really determined by our experiments)? (4) What other physical parameters involving the quasi-Ge parameters has been measured and can be used in our analysis?

### B. 1. Preliminary Analysis

(1) From the spectra and point plots we can get  $E_g$  directly. This is done by extrapolating each family of points in a point-plot (corresponding to the same minimum at different magnetic field values) to  $H=0$ . In each of the different polarization cases, we obtain nearly the same value. The energy thus obtained is actually  $E_g - E_B$ , i.e., reduced by exciton binding energy at zero field. This binding energy  $E_B$  is just  $R$ , the effective Rydberg for exciton (see Section A.4.).  $R$  is typically 3-5 meV for materials such as InP and GaAs and is expected to have the same typical value for our InGaAs and InGaAsP samples. We obtain directly

$$E_g - E_B \approx \begin{cases} 0.810 \text{ meV for T9-50} \\ 1.063 \text{ meV for Q9-18} \end{cases}$$

(2) The selection rules for RCP and LCP are different in the following manner. For LCP:  $a^\pm(n) \rightarrow a^C(n+1)$  and  $b^\pm(n) \rightarrow b^C(n+1)$  whereas for RCP:  $a^\pm(n) \rightarrow a^C(n-1)$  and  $b^\pm(n) \rightarrow b^C(n-1)$ . It is important to recall that for the heavy hole (-) series  $n \geq 1$  and for the light hole (+) series  $n \geq -1$ .

In view of these facts the two lowest energy heavy hole transition for the LCP case are  $a^-(1) \rightarrow a^C(2)$  and  $b^-(1) \rightarrow b^C(2)$ . The corresponding transition energies in most semiconductors and certainly in the binary semiconductors InP, InAs, GaAs are higher than those for the four lowest light hole transitions, namely  $a^+(-1) \rightarrow a^C(0)$ ,  $b^+(-1) \rightarrow b^C(0)$ ,

$a^+(0) a^c(1)$ , and  $b^+(0) b^c(1)$ . First, we note that the energies corresponding to  $a^+(-1)$ ,  $b^+(-1)$ ,  $a^-(1)$ , and  $b^-(1)$  lie close to each other and indeed, we can observe this directly from our data. Secondly, the Landau level spacings of the conduction bands are larger than those of the light hole band (and more so compared to those of the heavy hole band). This is because  $m_c < m_+ \ll m_-$ . Thirdly, the g-factor in these materials under study is expected to be small compared to  $m/m_c$  (since these are not small gap materials). The above can be checked from the formulas in Chapter II using approximate band parameters.

Hence for the LCP, the first six lowest transitions are expected to be

- 1, 2)  $a^+(-1) \rightarrow a^c(0)$  and  $b^+(-1) \rightarrow b^c(0)$
- 3, 4)  $a^+(0) \rightarrow a^c(1)$  and  $b^+(-1) \rightarrow b^c(1)$
- 5, 6)  $a^-(1) \rightarrow a^c(2)$  and  $b^-(1) \rightarrow b^c(2)$

For the RCP transitions on the other hand the first two lowest transitions have to be  $a^-(1) a^c(0)$  and  $b^-(1) b^c(0)$ . The next higher transitions are  $a^-(2) a^c(1)$ ,  $b^-(2) b^c(2)$ ,  $a^+(1) a^c(0)$  and  $b^+(1) b^c(0)$ .

- 1, 2)  $a^-(1) \rightarrow a^c(0)$  and  $b^-(1) \rightarrow b^c(0)$

For Voigt configuration with  $\vec{E} \parallel \vec{H}$  the lowest two transitions have to be  $b^-(1) a^c(0)$  and  $a^+(-1) b^c(0)$ .

The spectra for the ternary sample T9-50 clearly shows that

the first two transitions are very close to each other compared to their energy spacing with the next higher transitions. In fact, these two lowest transitions are expected to be  $a^+(-1) a^c(0)$  and  $b^+(-1) b^c(0)$ . Smallness of the energy spacing suggests that  $g_c + g_+$  is a small quantity ( $g_+$  is the g-factor of the light hole). In addition, note the energy difference  $E[a^+(-1) \rightarrow a^c(0)] - E[a^+(-1) \rightarrow b^c(0)] = \mu_B H g_c = E[b^-(-1) \rightarrow a^c(0)] - E[b^-(-1) \rightarrow b^c(0)]$ . Comparing the lowest transitions in the Voigt configuration with the lowest transition in the RCP and with the two close lying transitions in the LCP case, we see that indeed  $g_c \mu_B H$  is much smaller than  $\hbar \omega_c = \left(\frac{m}{m_c}\right) (2\mu_B H)$  as we pointed out earlier.

In summary, upon direct examination of our spectra, we can assert that the g factors for the conduction and light hole as well as the heavy hole are much smaller than  $m/m_c$ .

(3) The  $\vec{E} \parallel \vec{H}$  Voigt configuration spectra and the RCP spectra show much less structure than the LCP spectra as seen in Figures III-3 through III-9. This suggests that light hole transitions are strongest in the LCP polarization. Therefore, for our preliminary analysis we can assume that the minima which appear in the RCP and the Voigt  $\vec{E} \parallel \vec{H}$  spectra are mainly due to heavy-hole to conduction band transitions. We can then use these spectra to obtain an initial estimate for  $(1/\mu_-) \equiv (1/m_c) + (1/m_-)$  following a method similar to those used in Refs. 1, 2, and 17 and described in Appendix C. According to this for each polarization configuration and each H-orientation we can plot  $\epsilon(n)$  vs.  $2n\mu_B H$ . Here  $\epsilon(n) \equiv (1/2\mu_B H) [E(n) - E(n-1)]$  is the spacing between two adjacent transitions for a given H, in units of

$2n\mu_B H$ ,  $n$  being the conduction band Landau quantum number of the higher transition. According to the description in Appendix C a straight line drawn through these points (with a given light polarization and H-orientation) by the method of least squares fit intersects the  $(2n\mu_B H)=0$  axis at a value equal to  $(1/\mu_-) \equiv (1/m_c) + (1/m_-)$ . The slope of this line also gives the measure of nonparabolicity of the conduction band as explained in Appendix C. When this preliminary analysis was performed for the sample T9-50 we obtained somewhat different values for  $(1/\mu_-)$  for the [110] and [001] orientations indicating that the anisotropy factor  $\gamma_3 - \gamma_2 \neq 0$ . We obtained  $(1/\mu_-)_{[110]} \sim 25$ , and  $(1/\mu_-)_{[100]} \sim 26$  for T9-50 and  $(1/\mu_-) \sim 19$  for Q9-18 as preliminary values.

### B. 2. Band Parameters for Q9-18

In this section we present analysis and results for the Voigt  $\vec{E} \parallel \vec{H}$  magnetoabsorption spectra of the quaternary sample Q9-18 ( $\text{In}_{0.75}\text{Ga}_{0.25}\text{As}_{0.52}\text{P}_{0.48}$ ), which was presented earlier.<sup>26</sup>

1. As seen from Table IV-2 the heavy-hole mass  $m_{hh}$  shows only a small variation between the binary compounds. We have used  $m_{hh} = 0.45m$  ( $m_{hh} = m_{[100]}$  the heavy hole-mass along the [100] direction). However, varying  $m_{hh}$  between 0.04  $m$  and 0.05  $m$  would change electron and light hole masses by less than 3%.

2. The value of  $E_g = 1.066$  eV was determined from extrapolating the experimental data (1.063 eV) and corrected for the exciton binding energy at  $H=0$ ,  $E_B \approx 3$  meV. From absorption measurements made on a similar

alloy, we expect the room temperature energy gap to be about 1.00 eV.

3.  $\Delta=0.25$  eV was chosen from a linear interpolation using values in Table IV-1, however, varying between 0.2 and 0.3 eV changes the deduced electron effective mass by less than 0.5% and the light-hole mass by less than 3%. Very recently, measurement of  $\Delta$  for a number of quaternaries were performed by Herman, Lampel and Pearsall.<sup>24</sup> Interpolating their values for  $y=0.34$  and  $y=0.61$  we would get  $\Delta=0.23$  eV for our quaternary sample.

4. The anisotropy factor  $\gamma_3-\gamma_2$  was taken to be 0.7. This is predicted by Lawaetz<sup>25</sup> for the binary compounds. However, choosing  $\gamma_3-\gamma_2=0$  changes the deduced electron and the light hole mass by less than 0.15%.

5. The Kane parameter  $D_k$ , which is expected to be very small is taken to be zero for the binary semiconductors in the literature. We follow suite: this gives

$$\kappa = \gamma_3 + \frac{2}{3} \gamma_2 - \frac{1}{3} \gamma_1 - \frac{2}{3}$$

6.  $q$ , and  $N_1$  are expected to be very small (see Appendix B). These are set to be zero. In fact our fits, and our band parameters are very insensitive to  $q$  as large as  $\sim 0.5$  and  $N_1$  as large as  $\sim -0.1$ .

7.  $F$  is taken to be zero in this analysis. In other words,  $E_p$  was determined by assuming that the curvature of the  $\Gamma_6$  conduction band at  $\vec{k}=0$  comes entirely from the interaction with the  $\Gamma_8$  and  $\Gamma_7$

valence bands.  $E_p$  is expected to increase by 20% when the interaction with the  $\Gamma_8$  and  $\Gamma_7$  conduction bands due to admixing of the states by the antisymmetric potential is taken into account (i.e.,  $F \neq 0$ ).

8. Exciton corrections were taken into account following the discussion presented earlier. We obtained the following band parameters:  $E_g = 1.066$  eV,  $\Delta = 0.25$  eV,  $E_p = 17.6$  eV,  $m_c = 0.0608 m$ ,  $m_{hh} \equiv m_{[100]} = 0.45m$ ,  $m_{\rho h} = 0.078m$ ,  $\gamma_1 = 2.06$ ,  $\gamma_2 = -0.35$ ,  $\gamma_3 = 0.35$ , and  $\kappa = -1.234$ .

These values for  $\kappa$  and  $\gamma_3$  give  $q=0.02$  (see Appendix B) which indeed is small and has no influence on the fit, justifying  $q \approx 0$  assumption. Also from Appendix B, we see that  $-0.05 \leq N_1 < 0$ . The values of  $N_1$  in this range were seen not to influence the fit, only the reduced  $g_c$  by less than 0.2.

For various values of  $m_{hh}$ , the values obtained for  $(1/\mu_-)$  and  $(1/\mu_+)$  fall within a very narrow range. This is a very strong advantage of interband magnetoabsorption. Since  $m_{hh}$  turns out to be much larger than  $m_c$  these reduced masses are not very sensitive to  $m_{hh}$ , and these experiments can determine  $m_c$  within a narrow range. The values obtained from the above parameters are

$$\frac{m}{\mu_+} \equiv m \left( \frac{1}{m_c} + \frac{1}{m_+} \right) = 29.31$$

and

$$\frac{m}{\mu_-} \equiv m \left( \frac{1}{m_c} + \frac{1}{m_-} \right) = 18.65$$

We reported the above results in Refs. 26 and 27. (Figures III-3 and IV-1).

In a second attempt, we relaxed the restriction  $E_g=1066$  meV and used the minimization routine with the previously mentioned restrictions, this time, however, letting  $E_g$  vary as well. A slight improvement (DRMS = 2.06 meV per point as compared to the earlier value of 2.23 meV) was achieved with  $E_g=1064.28$  meV,  $E_p=17.985$  meV,  $\gamma_1=2.254$ ,  $\gamma_2=-0.251$ ,  $\gamma_3=0.449$ ,  $\beta=1.136$  giving  $m_c=0.0594m$  and  $m_+=0.0738m$  with  $\frac{m}{\mu_+}=30.37$  and  $\frac{m}{\mu_-}=19.05$ , an increase of 3.5% and 2.5% respectively. This value for  $(m_c/m)$  is 2.2% lower than the one we reported, well within experimental errors.

The recent measurement of  $m_c=0.0603m$  of Nicholas, et al<sup>28</sup> for a sample with  $y=0.53$  using cyclotron resonance is in excellent agreement with our result. This indicates the usefulness of interband magneto-optical measurements even though there are 10 band parameters involved and not all are known and even though some cannot be measured or deduced precisely. Reference 28, which uses intraband methods such as cyclotron resonance, magnetophonon effect, and Shubnikov de-Haas effect represents results of the most comprehensive intraband measurements of  $m_c$  for the whole range of  $y$  and suggest very strongly a linear dependence of  $m_c$  upon  $y$  in  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  samples lattice matched to InP. For a review of the reports on  $m_c$  dependence on  $y$  as evolved in time see Chapter I and references therein. Table IV-7 summarizes the results for  $m_c/m$  given in Ref.28.

### B.3 Band Parameters for Q9-18: Including Faraday Configuration Measurements

In order to make our study of the sample Q9-18 more complete it was decided also to make Faraday configuration interband magnetoabsorption measurements. Figures III-4 and III-5 give such spectra for RCP and LCP configurations with  $\vec{H} \parallel [100]$  for  $H=143.9$  kOe

The quasi-Ge analysis was carried out this time by including the data from the Voigt  $\vec{E} \parallel \vec{H}$  and the Faraday RCP and LCP spectra. Using the band parameters obtained for the Voigt data, we again obtained good fits, showing that these band parameters are consistent with the additional data taken on the Faraday configuration.

Having many more data points, we decided to run over minimization procedure again to see if new values for the parameters could be found which could improve the fits. This time with minimization routine we made the following constraints:

1) As before we assumed  $m_{hh}=0.45m$ , however, values of  $m_{hh}=0.5$  were also used which brought about very little change in the deduced band parameters, as was also the case before.

2)  $\Delta$  has been measured to be  $\sim 0.25$  eV by Nishino, et al<sup>29</sup> in a sample with similar composition using electroreflectance at 77K. From measurements of Ref. 24,  $\Delta$  is expected to be  $\sim 0.23 \pm 0.01$  eV. We used  $\Delta=0.24$  eV (as well as 0.25 and 0.23 eV). This variation in  $\Delta$  introduces a very small (<1%) uncertainty in the results.

3) Again  $D_K=0$  was used, which gives  $\kappa$  in terms of the  $\gamma$ 's.

4)  $q$  and  $N_1$  were related to the other parameters (see Appendix B). The range of values for  $q$  is close to zero and its effect on the band parameters is extremely small.  $N_1$  ranges between 0 and -0.07 and only affects the value of  $g_c$  by at most -0.2.

5) In each minimization trial a fixed value of  $F$  was chosen. These values were  $F=0, -0.5, -1, -1.5, -2, -2.5, -3, -3.5$ .  $N_1$  was related to  $F$  as in Appendix B.

6) In one series of runs  $\gamma_3 - \gamma_2 = 0.7$  was fixed. In another series of runs no restriction was imposed on  $\gamma_3 - \gamma_2$ . Another series of runs can be suggested which chooses a different fixed value for  $\gamma_3 - \gamma_2$ . We chose 0.7 since this seems to be the value most representative of the binaries.

7) In summary, in each minimization attempt,  $\Delta, F, m_{hh}, N_1$  were fixed, and  $E_g, E_p, \gamma_1, \gamma_2, \gamma_3, \kappa,$  and  $q$  were allowed to vary subject to the following constraints:

$$(1) \quad -\frac{1}{4} \gamma_1 + \frac{1}{2} \gamma_2 + \frac{3}{4} \gamma_3 - \frac{3}{4} \kappa = \frac{1}{2} \quad (4-14)$$

$$(2) \quad \gamma_1 - \frac{5}{4} \gamma_2 - \frac{3}{4} \gamma_3 \cong \frac{m}{m_{hh}} \quad (4-15)$$

$$(3) \quad -(0.011) \gamma_3 + (0.011) \kappa + q = -0.0055 \quad (4-16)$$

$$(4) \quad \gamma_3 - \gamma_2 = 0.7 \quad (4-17)$$

Where Eq.(4-17) was relaxed in one series of runs. For Eq.(4.16) see Eqs.(B-21) and (b-25). For Eq.(4-15) we note that  $m_{hh} = m_{-}[100]$  and according to Eq.(2-38)  $\frac{m}{m_{-}} \cong \gamma_1 - \frac{1}{2}(\gamma' + 3\gamma'')$  where  $\gamma'$  and  $\gamma''$  are given by Eqs.(2.23). For [100] direction  $\theta = \frac{\pi}{2}$  and  $\phi = \frac{\pi}{4}$  giving  $f(\theta, \phi) = 1$  and hence  $\gamma' = \gamma_2$  and  $3\gamma'' = \frac{3}{2}\gamma_2 + \frac{3}{2}\gamma_3$ , resulting in Eq.(4-15).

Table IV-3 shows results obtained for Q9-18 using the minimization routine with exciton corrections using the Voigt  $\vec{E} || \vec{H}$ , RCP and LCP spectra all with  $\vec{H} || [100]$ . In the minimization routine the following parameters were fixed  $\Delta = 0.24$  eV,  $\gamma_3 - \gamma_2 = 0.7$ ,  $q = N_1 - 0$ .  $m_{hh} = m_{-}[100] = 0.45m$ .  $F$  was also fixed and results were obtained for various values of  $F$ . Plots were made using parameters for  $F=0$  and for  $F=-2.381$ . The latter corresponds to  $E_p = 23.1$  which is obtained from the linear interpolation between the binaries InAs, GaAs, InP with  $E_p$  taken from Ref.30 which uses measured values of  $g_c$  and  $m_c$  to deduce  $E_p$  (see Appendix B and Table B-1). Plots corresponding to  $F=-2.381$  are presented in Figures IV-2 and IV-3. Those generated with  $F=0$  (first row of Table IV-3) turn out to be virtually identical to those corresponding to  $F=-2.381$  for all three polarizations (Voigt  $E \parallel H$ , RCP and LCP). In other words whether we choose to ignore the effect of the higher bands on the curvature at the bottom of the conduction band ( $F=0$ ) or include the effect (with  $E_p$  assumed to have the linear interpolation value) other parameters will adjust to give nearby identical fits. In Table IV-3 we have also calculated the value of  $\alpha$  which is a measure of the nonparabolicity of the conduction band (see Appendix C) using the

band parameters for each fit. The variation of  $\alpha$  for  $F=0$  to  $F=-3.5$  is from 0.94 to 0.846, a 12.5% decrease. From  $F=0$  to  $F=2.381$  ( $E_p=23.1$ )  $\alpha$  decreases by 0.049 or 5.1%. For  $H=150kOe$  on  $n=7$  the difference between the energies of transition to  $a^C(n)$  is calculated to be  $\sim 3$  meV using Eq.(C-18). Numerical calculations using the quasi-Ge Hamiltonians show an even better agreement to within  $\sim 0.5$  meV. This shows that the nonparabolicity of the conduction band is not large enough to narrow down the range of  $E_p$  in these materials, in contrast with the small gap materials such as InSb. Thus interband magneto-optical measurements involving  $\Gamma_8^V$  and  $\Gamma_6^C$  bands alone cannot determine  $E_p$  precisely in the quaternaries and this suggests the usefulness of P measurements involving  $\Gamma_7^V \rightarrow \Gamma_6^C$  transitions, or direct measurement of  $g_c$  to obtain  $E_p$  (see Ref.30 and Appendix B). Another feature apparent from Table IV-3 is the fact that  $m_c$ ,  $m_+$  (or  $\mu_+$ ,  $\mu_-$ ),  $\gamma_1^L$ ,  $\gamma_3^L$  and  $\kappa^L$  vary very slightly although  $E_p$  varies from 17.91 to 25.38. Varying  $m_{hh} \equiv m_- [100]$  between from 0.45m to 0.4m or to 0.5m changes  $\mu_-$  and  $\mu_+$  by less than 0.1%. As a result  $m_c$  and  $m_+$  are determined to within  $\pm 1.5\%$ . In the case of Q9-18 measurements were done with  $\vec{H} || [100]$ , so the anisotropy factor  $\gamma_3 - \gamma_2 = 0.7$  is used from comparison with T9-50 and the binaries InAs, GaAs and InP. It turns out that when the restriction on  $\gamma_3 - \gamma_2$  is removed the value obtained from the minimization routine is  $\gamma_3 - \gamma_2 = 0.35 \pm 0.05$ ; nevertheless the values obtained for  $m_c$  and  $m_+$  were the same within 0.1% or better for  $\gamma_3 - \gamma_2 = 0.7$  or 0.35.

Table IV-3 shows that the only precise measurement of  $g_c$  can narrow down  $E_p$ . Figures IV-1 through IV-3 show experimental points

corresponding to the  $T(H)/T(0)$  minima the lines are transition energies as a function of  $H$  calculated using the quasi-Ge Hamiltonians with exciton corrections. Solid lines represent heavy hole to conduction band transitions and dashed lines, light hole to conduction band. The transitions are identified in Tables IV-4 and IV-5.

In summary for  $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}_{0.52}\text{P}_{0.48}$  (Q9-18) we have obtained

$$E_g = 1065 \pm 1 \text{ meV} \quad (m/\mu_+) = 29.5 \pm 0.5, \quad (m/\mu_-) = 18.8 \pm 0.5.$$

$$m_c/m = 0.0602 \pm 0.001, \quad m_+/m = 0.078 \pm 0.001,$$

$$\gamma_1^L = 7.5 \pm 0.2, \quad \gamma_3^L = 3.1 \pm 0.1, \quad \kappa^L = 1.5 \pm 0.1. \quad \text{Assuming}$$

$$m_{hh} \equiv m_{-}[100] = 0.45 \pm 0.05, \quad \Delta = 0.24 \pm 0.01 \text{ eV} \text{ and } F = 0 \text{ to } -3.5. \text{ We}$$

assumed  $\gamma_3 - \gamma_2 = 0.7$  although the values given above remain rather insensitive to changes equal to as much as 0.35 in  $\gamma_3 - \gamma_2$ . For

$$F = 0 \text{ to } -3.5: E_p \cong 17.5 \text{ to } 25.8 \text{ eV, and } g_c \cong -0.05 \text{ to } -1.5$$

Preliminary measurements of  $g_c^{32}$  suggests that  $E_p$  is close to the linear interpolated value of 23.1 eV. (See also Table IV-6).

The value for  $\bar{\beta}$  which we have calculated from our band parameter (Table IV-3) lies very close to the linear interpolation between those values for InP and  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  (ternary). The value of  $\bar{\beta}$  for the ternary has been measured by Hermann et al<sup>24</sup> who use optical pumping measurements and agrees very well with that calculated from our band parameters for the Ternary. (See also Table IV-6).

Here

$$\bar{\beta} \equiv \frac{1}{3} \frac{3(m/\mu_+) + (m/\mu_-)}{(m/\mu_+) - (m/\mu_-)}$$

The conduction effective mass values for  $y=0$  to  $y=1$  reported in Ref.28 and obtained from cyclotron resonance and magnetophonon resonance are seen to lie on a straight line (see Table V-7). This is in excellent agreement with our results for both the quaternary Q9-18 ( $x=0.25$ ,  $y=0.52$ ) and the ternary T9-50 ( $x=0.47$ ,  $y=1$ ). The above discussion indicates that (1) interband magneto-optical measurements, and (2) the interband measurements such as cyclotron and magneto phonon resonance and (3) optical pumping measurements (including electron spin resonance) are complementary methods for measuring band parameters of semiconductors. It is interesting to note that they all fall in the category of magneto-optics.

#### B. 4. Band Parameters for T9-50

Analysis of the data for T9-50 follows exactly the same line as presented for Q9-18. Qualitatively, many of the assertions about Q9-18 hold for T9-50. Tables similar to Table IV-3 were generated and the following results were obtained:

1) In what follows the minimization routine was run each time with the parameters  $\Delta$ ,  $q$ ,  $N_1$ , were kept fixed.  $E_g$ ,  $E_p$ ,  $\gamma_1$ ,  $\gamma_2$ ,  $\gamma_3$ , and  $\kappa$  were free to vary subject to  $D_K=0$  and  $m_-$ =fixed. We obtained the following results

(a)  $\Delta=0.35$  eV vs.  $\Delta=0.36$  eV: Optimization in each gave

same DRMS. The following changes were observed:

$m_c$  by  $\lesssim 0.1\%$ ,  $\mu_-$  by  $\lesssim 0.2\%$ ,  $g_c$  by  $\lesssim 0.5\%$ .

$\mu_+$  by  $\lesssim 0.1\%$  and  $E_g$ ,  $E_p$  and  $(\gamma_3-\gamma_2)$  by  $\lesssim 0.005\%$ .

(b)  $N_1=0$  vs.  $N_1=-0.03$ : In the case  $g_c$  changed by 0.12 and  $(\gamma_3-\gamma_2)$  by 0.2%. The other parameters changed by less than 0.005%.

(c)  $q=0$  vs.  $q=0.03$ : In this case  $(\gamma_3=\gamma_2)$  changed by  $\lesssim 0.4\%$   $m_+$  and  $\mu_+$  changed  $\lesssim 0.05\%$  and the other parameters by less than 0.001%.

Therefore, we note that whether we set  $q=N_1=0$ , or we use their estimated values (Appendix B), no difference is made in the fits, and we might as well set them equal to zero.

2) In what follows we run the minimization routine with  $m_- = 0.5 m$ ,  $\Delta = 0.35$  eV,  $q = N_1 = D_K = 0$ . We then run the optimization routine with  $F = 0, -0.5, -1, -1.5, -2, -2.2, -2.4, -2.5, -3, -3.5$ . We observed that DRMS varies from 2.687 meV for  $F=0$  to 2.676 for  $F=-2$  through  $F=-2.5$  and to 2.683 for  $F=-3.5$ . Hardly a decisive minimum to narrowly determine  $F$ . Considering light hole transitions only we still did not get a decisive minimum for DRMS to determine  $F$  narrowly.

(a) The value of  $E_p$  varies from 21.0687 eV to 27.0441 eV. The interpolated value of  $E_p = 25.35$  eV corresponding to  $F = 2.46$  give DRMS = 2.687 meV. We see that our measurements cannot precisely measure  $E_p$ . However, with  $N_1 = 0$ , the value of  $g_c$  changes from -3.2 to -4.67. If as in Appendix B we use

the estimated value of  $N_1=0.014F-0.02$  the range of  $g_c$  would be -3.3 to -4.95. Therefore, a measurement of  $g_c$  with good precision can determine  $E_p$ . (Refer to Table IV-8.)

(b) The value of  $E_g$  varies between 812.77 and 813.29 meV; also for  $m_-/m$  between 0.4 and 0.6 and a given  $F$ , optimal values of  $E_g$  varies by about 0.5 meV. Therefore, interband magnetoabsorption experiments yield  $E_g=813\pm 0.5$  meV.

(c) Again for  $F=0$  to -3.5 the minimization routine yielded 0.8035  $\gamma_3-\gamma_2$  0.751 for  $m_{hh}=0.5m$ . In fact for  $m_{hh}/m$  between 0.4 and 0.5, optimal values for  $\gamma_3-\gamma_2$  lie between 0.74 and 0.83. As mentioned before interband magnetoabsorption experiments determine  $\gamma_3-\gamma_2$  narrowly provided spectra are taken with  $\vec{H}$  along different crystal axes. In the case of T9-50, we had taken spectra with  $\vec{H}||[100]$  and with  $\vec{H}||[110]$ .

(d) The values for  $\mu_+/m$  and  $\mu_-/m$  are again narrowly determined by interband magnetoabsorption measurements. Again, with  $m_{hh}/m=0.5$ , as  $F$  was varied between 0 and -3.5,  $\mu_+/m$  changed from 0.02293 to 0.02318, a change of 0.3%. This gave  $43.14\leq m/\mu_+\leq 43.60$  similarly  $0.03848\leq \mu_-/m\leq 0.03799$  giving  $25.92\leq m/\mu_+\leq 26.32$ . For different values of  $m_-/m$  between 0.4 and 0.6 these values change by about  $\pm 0.2\%$ . It is also found that fits with values differing by  $\pm 1\%$  to  $\pm 2\%$  of these values although strictly not optimal in the

mathematical sense, still give fits quite as good. This means that

$$(m/\mu_+) = 43.4 \pm 1.0$$

$$(m/\mu_-) = 26.1 \pm 0.5$$

(e) For  $m_{hh}/m=0.5$  and  $F$  from 0 to  $-3.5$  the values for  $m_c/m$  changes from 0.04112 to 0.04181, i.e., by 2% whereas the value for  $m_+/m$  changes from 0.05186 to 0.05201, a mere 0.2%. For different values of  $m_{hh}/m$  between 0.4 and 0.6 and a given  $F$ ,  $m_c$  changes by 3%, and  $m_+$ , by 2%. Therefore our experiments give  $m_c/m = 0.0415 (1 \pm 5\%) = 0.0415 \pm 0.0015$  and  $m_{hh}/m = 0.0515 \pm 0.0015$ .

(f)  $\beta \approx 3 \pm 0.05$  in excellent agreement with Ref. 24.

$$(g) \quad \gamma_1^L \approx 10.6 \pm 0.2, \quad \gamma_2^L \approx 4.0 \pm 0.1, \quad \gamma_3^L = 4.8 \pm 0.1, \\ \kappa^L = 3.3 \pm 0.1.$$

TABLE IV-1 Binding energy  $E_B$  of the 1S state of a hydrogen-like atom (in units of the effective Rydberg R) vs. the reduced magnetic field  $\gamma$ , (see Text).

$\gamma$	$E_B$	$\gamma$	$E_B$	$\gamma$	$E_B$
0.0	1.000	1.5	1.869	23.4	4.629
0.025	1.025	1.6	1.906	25.0	4.733
0.05	1.049	1.7	1.941	30.0	5.031
0.075	1.072	1.8	1.975	34.95	5.293
0.1	1.095	2.0	2.041	40.0	5.535
0.15	1.139	2.2	2.103	45.0	5.754
0.2	1.181	2.4	2.162	50.0	5.957
0.25	1.220	2.5	2.191	55.0	6.146
0.3	1.258	2.6	2.218	62.91	6.422
0.4	1.329	2.8	2.272	69.9	6.645
0.5	1.394	3.0	2.323	83.88	7.048
0.6	1.454	3.5	2.444	97.0	7.384
0.7	1.511	5.0	2.750	100.0	7.519
0.8	1.564	7.5	3.152		
0.9	1.613	8.388	3.273		
1.0	1.661	10.0	3.474		
1.1	1.707	12.58	3.755		
1.2	1.749	15.0	3.985		
1.3	1.791	17.48	4.198		
1.4	1.831	20.0	4.392		

TABLE IV-2 Band parameters for binary semiconductors determined from interband magneto-optical measurements used to estimate band parameters for  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$ .

	InAs <sup>a</sup>	GaAs <sup>a</sup>	InP <sup>b</sup>
$E_g$ (eV)	0.41	1.52	1.42
$\Delta$ (eV)	0.38	0.34	0.11
$E_p$ (eV) <sup>c</sup>	20	22	17
$m_c/m_0$	0.024	0.067	0.079
$m_{hh}/m_0$	0.4	$0.45 \pm 0.07$	$0.45 \pm 0.05$
$m_{lh}/m_0$	0.026	0.082	0.12
$\gamma_3 - \gamma_2$	$0.7^d$	0.7	$0.7^d$

<sup>a</sup>From values quoted in Ref.6.

<sup>b</sup>Ref.23.

<sup>c</sup>These values for  $E_p$  are not deduced from direct measurements of  $g_c$  and  $m_c$ . Therefore these were not used in our actual calculations, instead, we used  $E_p$  values given in Ref.30 (see Table B-1).

<sup>d</sup>Ref.25.

Table IV-3

Band parameters obtained for the sample Q9-18 using the minimization routine with exciton corrections using data from the Voigt  $\vec{E} \parallel \vec{H}$ , RCP, and LCP spectra, all with  $\vec{H} \parallel [100]$ . In the minimization routine, the following parameters were fixed:  $\Delta = 0.24$  eV,  $\gamma_3 - \gamma_2 = 0.7$ ,  $q = N_1 = 0$ ,  $m_{hh} \equiv m_{-}[100] = 0.45$  m, and F.

F	DRMS (meV)	$E_g$ (meV)	$E_p$ (eV) $g_c$ †	$\gamma_1$ $\gamma_3$	$\gamma_1^L$ $\gamma_3^L, \kappa^L$	$m_c/m$ $m_+/m$	$\mu_+/m$ $m/\mu_+$	$\mu_-/m$ $m/\mu_-$	$\bar{\beta}$	$\alpha$ $(m/m_c)^{2\alpha}$
0	3.459	1064.29	17.9055 -0.064† -0.20 †	1.9485 0.2964	7.5565 3.1004 1.5152	0.05955 0.07757	0.03369 29.68	0.05259 19.015	3.377	0.964 271.86
-1.0	3.457	1064.35	20.1497 -0.32 -0.51	1.2343 -0.0607	7.5448 3.0945 1.5093	0.05963 0.07771	0.03374 29.64	0.05265 18.99	3.379	0.959 269.78
-2.0	3.458	1064.55	22.3021 -0.57 -0.82	0.5489 -0.4034	7.5262 3.0853 1.5001	0.06001 0.07787	0.03389 29.51	0.05295 18.86	3.371	0.931 258.61
-2.381*	3.459	1064.66	23.0996 -0.66 -0.93	0.2956 -0.5301	7.5278 3.0860 1.5008	0.06023 0.07792	0.03397 29.44	0.05312 18.825	3.365	0.915 252.12
-3.0	3.468	1064.89	24.3700 -0.81 -1.11	-0.1064 -0.7311	7.5219 3.0831 1.4979	0.06067 0.07799	0.03413 29.30	0.05346 18.71	3.354	0.880 239.19
-3.5	3.479	1065.10	25.3764 -0.93 -1.25	-0.4225 -0.8891	7.5193 3.0818 1.4966	0.06111 0.7803	0.03427 29.18	0.05381 18.58	3.338	0.846 226.59

\*Parameters used in Figs. IV-4 and IV-5. Value of  $E_p$  corresponds to the linear interpolation (see Table B-1).

†The lower value for  $|g_c|$  corresponds to  $N_1 = 0$ , the higher value corresponds to  $N_1 = 0.14 F - 0.034$  as in Table B-2.  $\alpha$  is a measure of the nonparabolicity of the conduction band given by Eq. (C-18) in Appendix C.

$$\bar{\beta} = \frac{1}{3} \frac{3(m/\mu_+) + (m/\mu_-)}{(m/\mu_+) - (m/\mu_-)}$$

TABLE IV-4 Identification of Interband Transition Lines in the Voigt Configuration (i.e.  $\vec{k} \perp \vec{H}$ ) for  $\vec{E} \parallel \vec{H}$ .

Label	Transition	Label	Transition	Label	Transition
1	$b^-(1)a^c(0)$	11	$b^+(2)a^c(1)$	21	$b^+(4)a^c(3)$
2	$a^+(-1)b^c(0)$	12	$a^-(3)b^c(4)$	22	$a^-(6)b^c(7)$
3	$b^-(2)a^c(1)$	13	$b^-(5)a^c(4)$	23	$b^-(8)a^c(7)$
4	$a^+(0)b^c(1)$	14	$a^+(2)b^c(3)$	24	$a^-(7)b^c(8)$
5	$b^+(1)a^c(0)$	15	$b^+(3)a^c(2)$	25	$b^-(9)a^c(8)$
6	$a^-(1)b^c(2)$	16	$a^-(4)b^c(5)$	26	$a^+(4)b^c(5)$
7	$b^-(3)a^c(2)$	17	$b^-(6)a^c(5)$	27	$b^+(5)a^c(4)$
8	$a^+(1)b^c(2)$	18	$a^-(5)b^c(6)$	28	$a^-(8)b^c(9)$
9	$a^-(2)b^c(3)$	19	$b^-(7)a^c(6)$	29	$b^-(10)a^c(9)$
10	$b^-(4)a^c(3)$	20	$a^+(3)b^c(4)$		

TABLE IV-5 Identification of Interband Transitions in the Faraday Configuration (i.e.  $\vec{k} \parallel \vec{H}$ )

	<u>RCP</u>	<u>LCP</u>
1.	$a^-(1)a^C(0)$	$a^+(-1)a^C(0)$
2.	$b^-(1)b^C(0)$	$b^+(-1)b^C(0)$
3.	$a^+(1)a^C(0)$	$a^+(0)a^C(1)$
4.	$a^-(2)a^C(1), b^-(2)b^C(1)$	$b^+(0)b^C(1)$
5.	$a^-(3)a^C(2), b^-(3)b^C(2)$	$a^+(1)a^C(2)$
6.	$a^+(2)a^C(1)$	$a^-(2)a^C(3), b^-(2)b^C(3)$
7.	$a^-(4)a^C(3), b^-(4)b^C(3)$	$b^+(1)b^C(2)$
8.	$a^-(5)a^C(4), b^-(5)b^C(4)$	$a^-(3)a^C(4), b^-(3)b^C(4)$
9.	$a^+(3)a^C(2)$	$a^-(4)a^C(5), b^-(4)b^C(5)$
10.	$a^-(6)a^C(5), b^-(6)b^C(5)$	$b^+(2)b^C(3)$
11.	$a^-(7)a^C(6), b^-(7)b^C(6)$	$a^-(5)a^C(6), b^-(5)b^C(6)$
12.	$a^+(4)a^C(3)$	$a^-(6)a^C(7), b^-(6)b^C(7)$
13.	$a^-(8)a^C(7), b^-(8)b^C(7)$	$b^+(3)b^C(4)$
14.	$a^-(9)a^C(8), b^-(9)b^C(8)$	$a^-(7)a^C(8), b^-(7)b^C(8)$
15.	$a^+(5)a^C(4)$	$a^-(8)a^C(9), b^-(8)b^C(9)$
16.	$a^-(10)a^C(9), b^-(10)b^C(9)$	$b^+(4)b^C(5)$
17.	$a^-(11)a^C(10), b^-(11)b^C(10)$	$a^-(9)a^C(10), b^-(9)b^C(10)$
18.	$a^+(6)a^C(5)$	$a^-(10)a^C(11), b^-(10)b^C(11)$
19.	$a^-(12)a^C(11), b^-(12)b^C(11)$	$b^+(5)b^C(6)$
20.	$a^-(13)a^C(12), b^-(13)b^C(12)$	$a^-(11)a^C(12), b^-(11)b^C(12)$

Table IV-6

Optical Pumping Measurements in  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  Epitaxial Samples (After Ref. 24)\*

x	y	$E_g$ (eV)	$E_g + \Delta$ (eV)	$\Delta$ (eV)	$\bar{\beta}$	$m_c/m$	$m_+/m$	$g_c^a$
0	0	$1.423 \pm 0.0005^b$	$1.531 \pm 0.0025^b$	$0.108^b$	$4.1 \pm 0.5^c$	$0.079^b$	$0.12 \pm 0.01^b$	+1.24
0.16	0.34	$1.19 \pm 0.01$	$1.37 \pm 0.005^\dagger$	0.18	$4.2 \pm 0.4^\dagger$	$0.066^d$	$0.109$ $0.9^a$	+0.50
$0.26^a$	$0.60^a$	$1.035^a$		$0.25^a$			$0.072^a$	-1.25
0.30	0.61	$1.035 \pm 0.01$	$1.29 \pm 0.01$	0.255	$3.4 \pm 0.4$	$0.052^d$	$0.072 \pm 0.01$	
0.39	0.84	$0.875 \pm 0.01$	$1.18 \pm 0.01$	0.305		$0.046^d$	$0.061 \pm 0.007$	-3.0
0.47	1	$0.80 \pm 0.1$ $0.810$	$1.15 \pm 0.01^*$	$0.35$ $0.340$	$3.0 \pm 0.2^\dagger$	$0.041^d$	$0.051 \pm 0.005$	-4.2 $\pm$ 25%

\*Values in this table are obtained by Hermann, Lampel, and Pearsall<sup>24</sup> and at  $T = 1.7\text{K}$ , unless otherwise indicated.

<sup>†</sup>These results were the same at 1.7 K and 77 K.

<sup>a</sup>T.P. Pearsall, Private Communication.

<sup>b</sup>From Ref. 23.

<sup>c</sup>Calculated from Ref. 23.

<sup>d</sup>From Ref. 33.

TABLE IV-7 Conduction band effective mass obtained by cyclotron resonance and magnetophonon resonance for  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$ . (After Ref.28).

Alloy composition		Cyclotron <sup>†</sup> resonance	Magnetophonon <sup>†</sup> resonance	
			InP mode	InGaAs mode
x	y	$m_{\text{HF}}^*/m$	$m_{\text{HF}}^*/m$	$m_{\text{HF}}^*/m$
0.11	0.23	0.0693	0.071*	...
0.15	0.33	0.0666	...	...
0.25	0.53	0.0603	...	...
0.25	0.54	...	0.0602	0.0587
0.26	0.58	...	0.0585	0.0565
0.26	0.59	...	0.0583	0.0565
0.30	0.64	0.055	...	...
0.38	0.84	0.0468	0.0478	0.0468
0.41	0.91	...	...	0.0441
0.47	1.0	0.041*	...	0.043*

<sup>†</sup>  $m_{\text{HF}}^*$  ≡ High frequency or true "bare" mass

\* From Ref.33

Table IV-8

Band Parameter for T9-50, with  $\Delta = 0.35$  eV,  $q = 0$ ,  $N_1 = 0$ ,  $m_{-}[100]=0.5m$  kept fixed\*

Run	F	DRMS (meV)	$\gamma_3 - \gamma_2$	$E_g$ (meV)	$E_p$ (eV) $g_c$	$m_c/m$	$m_+/m$	$\mu_+/m$ $m/\mu_+$	$\mu_-/m$ $m/\mu_-$	$\gamma_1^L$ $\gamma_3^L$
1	22.6	0	2.687	0.8034	812.77 21.0687 -3.202	0.04112	0.05186	0.02293 43.60	0.03799 26.32	10.6406 4.8188
2	22.7	-0.5	2.683	0.7969	812.77 21.9711 -3.425	0.04112	0.05190	0.02294	0.03799	
3	22.8	-1.0	2.680	0.7907	812.80 22.856 -3.643	0.04115	0.05194	0.02296	0.03802	
4	22.9	-1.5	2.678	0.7844	812.85 23.7244 -3.856	0.04122	0.05197	0.02299	0.03808	
5	22.10	-2.0	2.676	0.7783	812.93 24.5765 -4.066	0.04132	0.05199	0.02302	0.03817	
6	22.10	-2.2	2.676	0.7758	812.97 24.9131 -4.148	0.04137	0.05200	0.02304	0.03821	
7	22.12	-2.4	2.676	0.7734	813.01 25.2472 -4.23	0.04143	0.05200	0.02306 43.365	0.03826 26.13	
8	22.13	-2.5	2.676	0.772	813.03 25.4134 -4.271	0.04146	0.0520	0.02307 43.35	0.03828 26.12	10.615 4.7868
9	22.14	-3.0	2.678	0.7657	813.15 26.2355 -4.472	0.04162	0.05201	0.02312	0.03842	
10	22.15	-3.5	2.683	0.7591	813.29 27.0441 -4.67	0.04181	0.05201	0.02318 43.14	0.03858 25.92	

\*This Table is the result of minimization routine with exciton corrections using the data for T9-50 taken in the following configurations: Faraday, RCP and LCP with  $\vec{H}||[100]$ , Voigt  $\vec{E}||\vec{H}$  and  $\vec{E}_\perp\vec{H}$  with  $H||[110]$ .

FIGURE IV-1 Point plot and fan chart (photon energy vs. magnetic field) for the magnetoabsorption spectra obtained in the Voigt configuration ( $\vec{k} \perp \vec{H}$ ) with  $\vec{E} \parallel \vec{H}$  for the sample Q9-18. Transmission minima at various magnetic fields are shown by the dots. Curves are calculated transition energies based on the quasi-Ge analysis with exciton corrections. Solid lines represent the heavy hole to conduction band transitions, dashed lines represent the light hole to conduction band transitions. The transitions are numbered according to Table IV-4 in the order of increasing energies as follows: 1,2,3,5,4,6,7,8,11,9,10,12,13,14,15,16,17, 20,21,18,19.

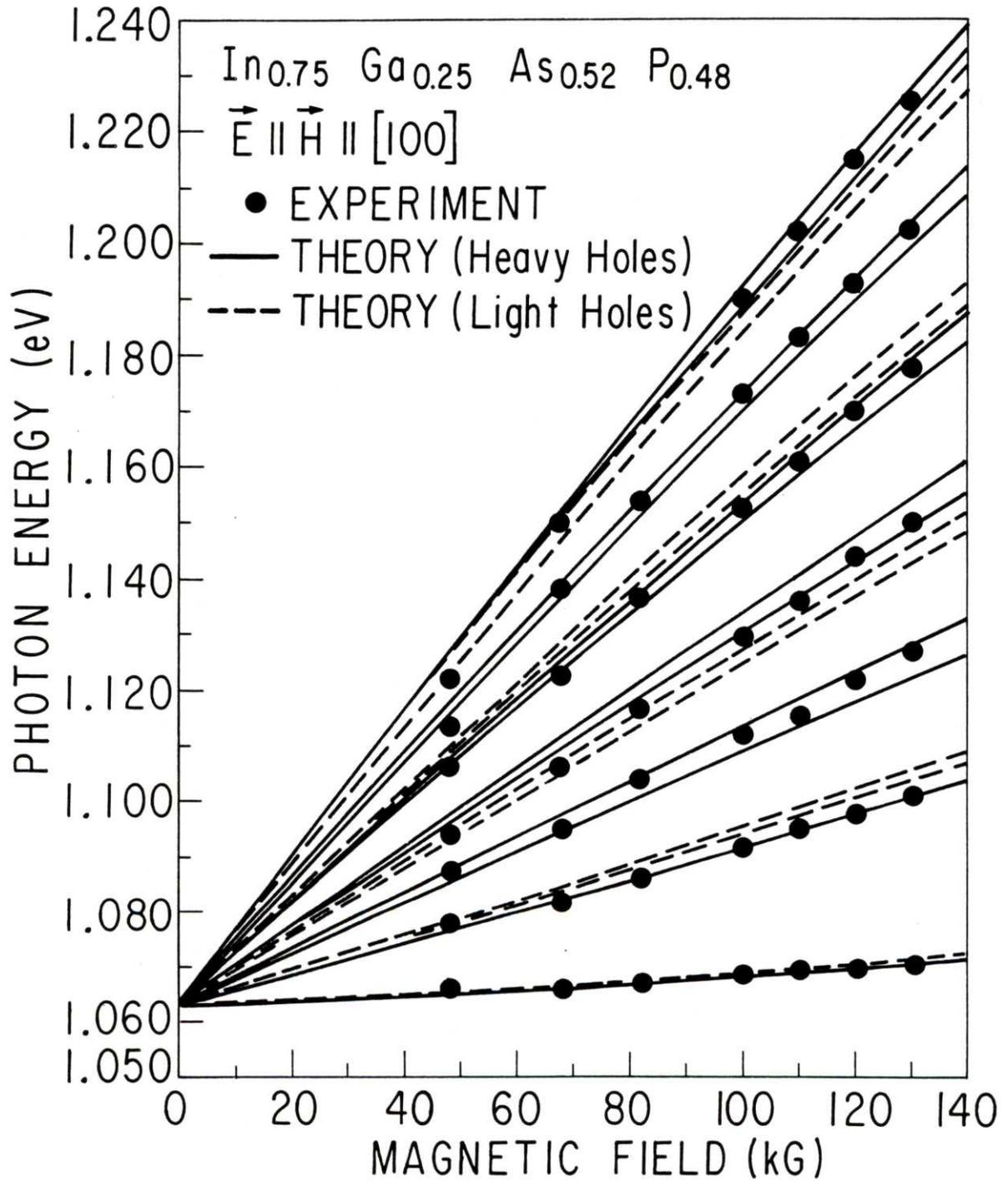


FIGURE IV-2 Point plot and fan chart (photon energy vs. magnetic field) for the interband transitions in the Faraday configuration ( $\vec{k} \parallel \vec{H}$ ) with RCP polarized light for Q9-18. Dots represent experimental data (minima in transmission spectra). Lines represent calculated transition energies based on the quasi-Ge analysis with exciton corrections and are numbered according to Table IV-5. The solid lines represent the heavy hole to conduction band transitions. The dashed lines represent transition from the light hole to the conduction band.

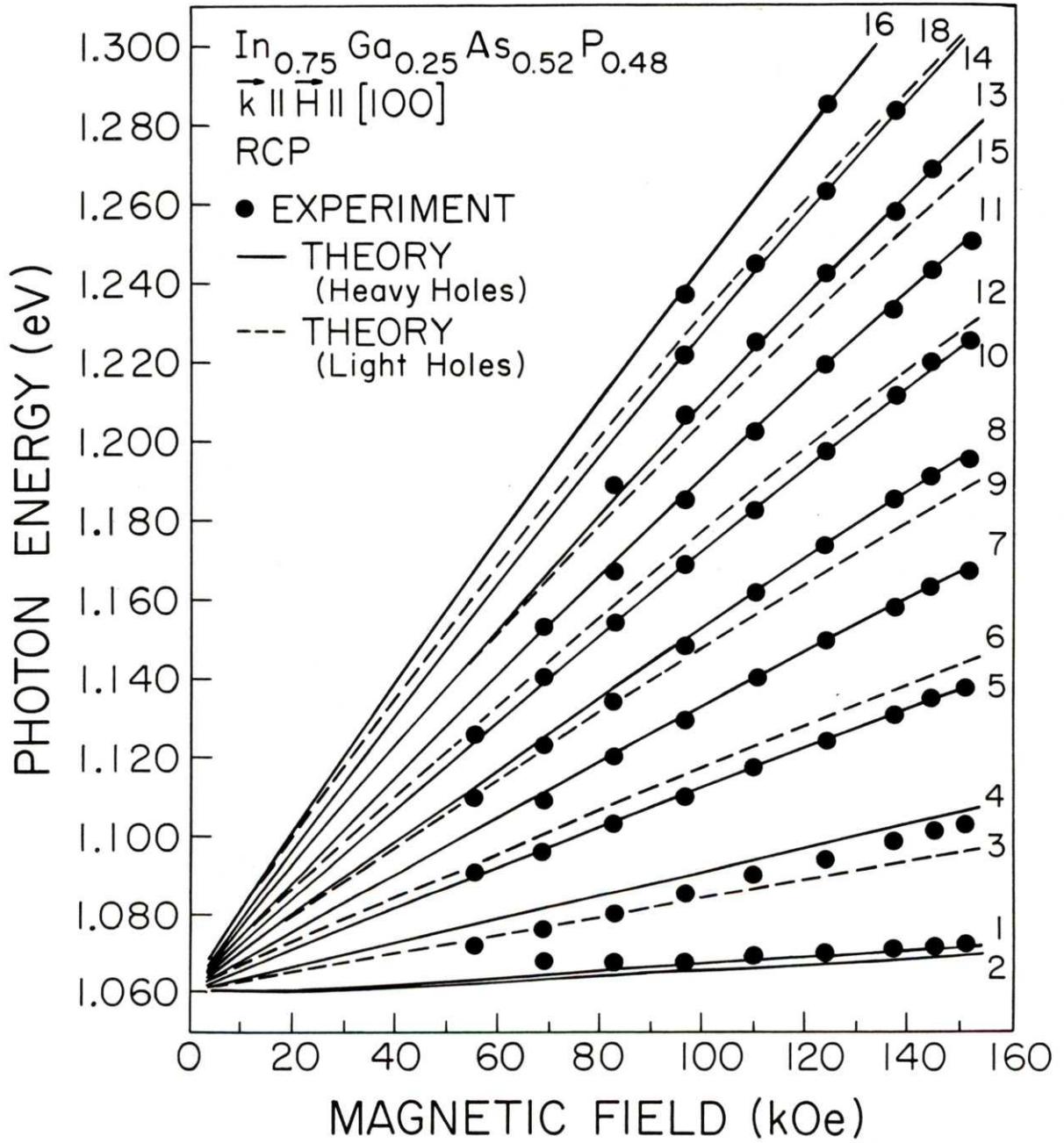


FIGURE IV-3 Point plot and fan chart (photon energy vs. magnetic field) for the interband transitions in the Faraday configuration ( $\vec{k} \parallel \vec{H}$ ) with LCP polarized light for Q9-18. The calculated transition lines are labeled according to Table IV-5. The unnumbered line corresponds to the two close-lying transitions  $a^-(1)a^C(2)$  and  $b^-(1)b^C(2)$ .

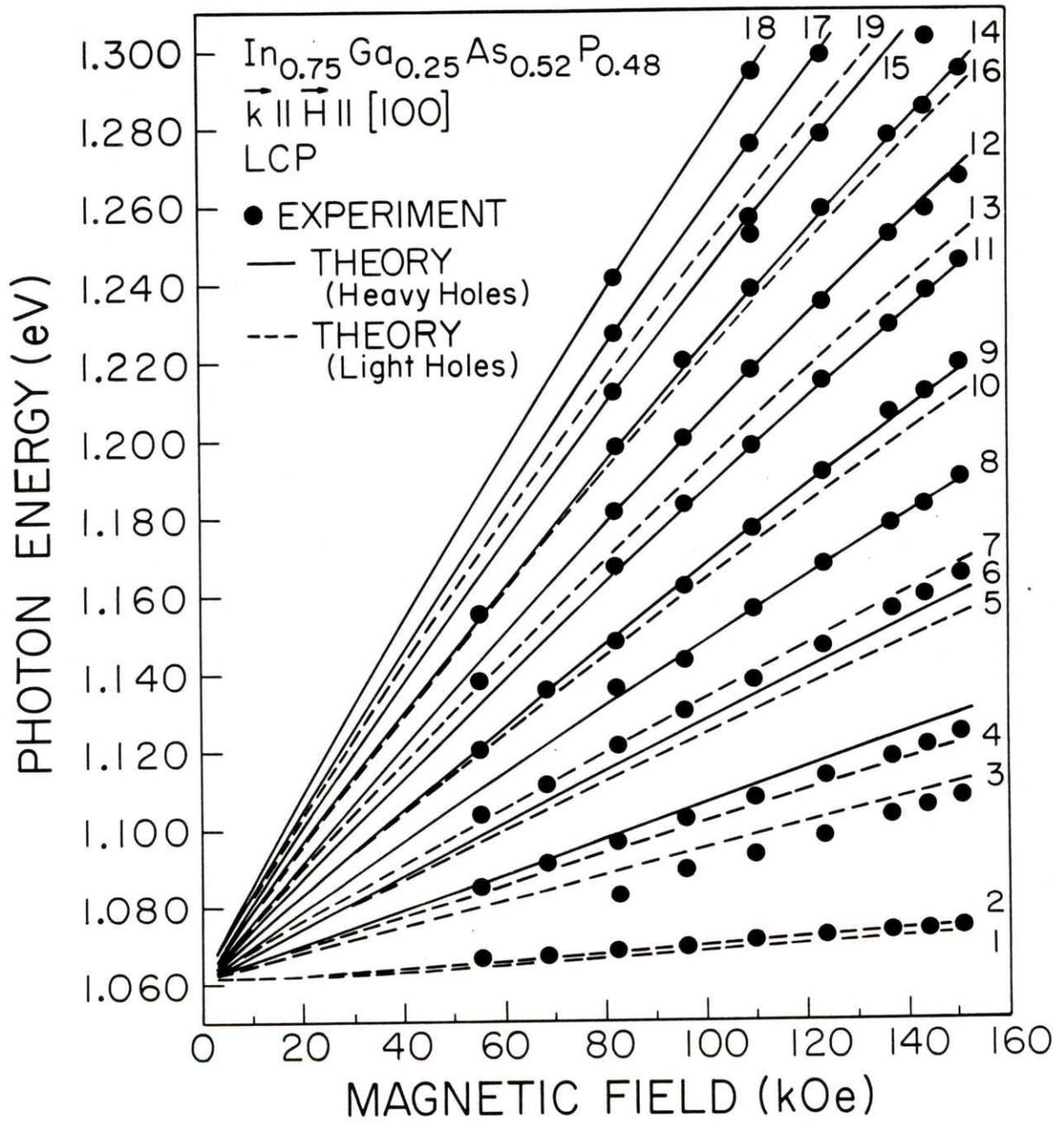


FIGURE IV-4 Point plot and fan chart (photon energy vs. magnetic field) for the interband transitions in the Voigt configuration ( $\vec{k} \perp \vec{H}$ ) with  $\vec{E} \parallel \vec{H}$  for the sample T9-50. Transitions are numbered according to Table IV-4.

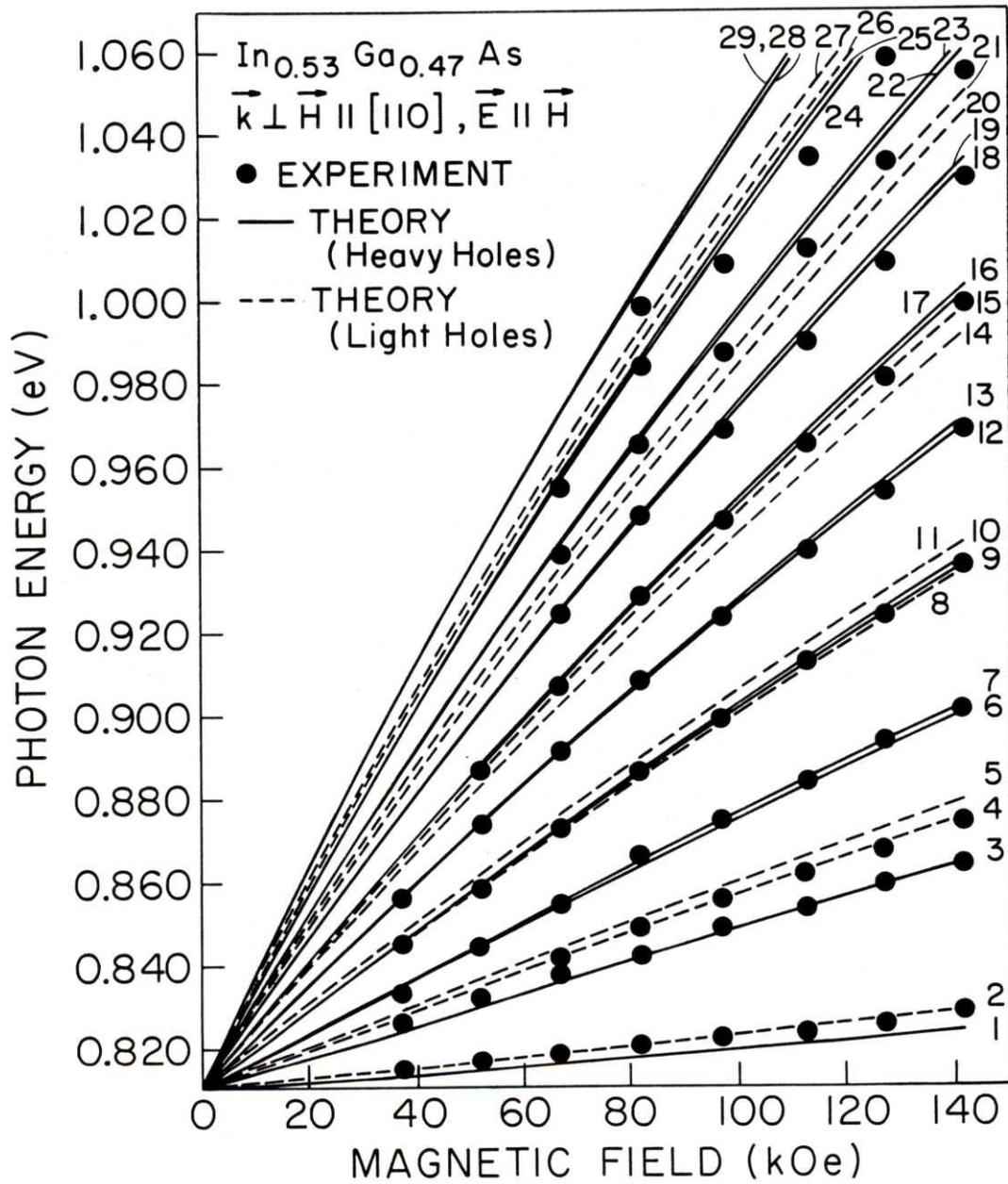


FIGURE IV-5 Point plot and fan chart (photon energy vs. magnetic field) for the interband transitions in the Faraday configuration ( $\vec{k} \parallel \vec{H}$ ) with RCP polarized light for T9-50. The transitions are numbered according to Table IV-5.

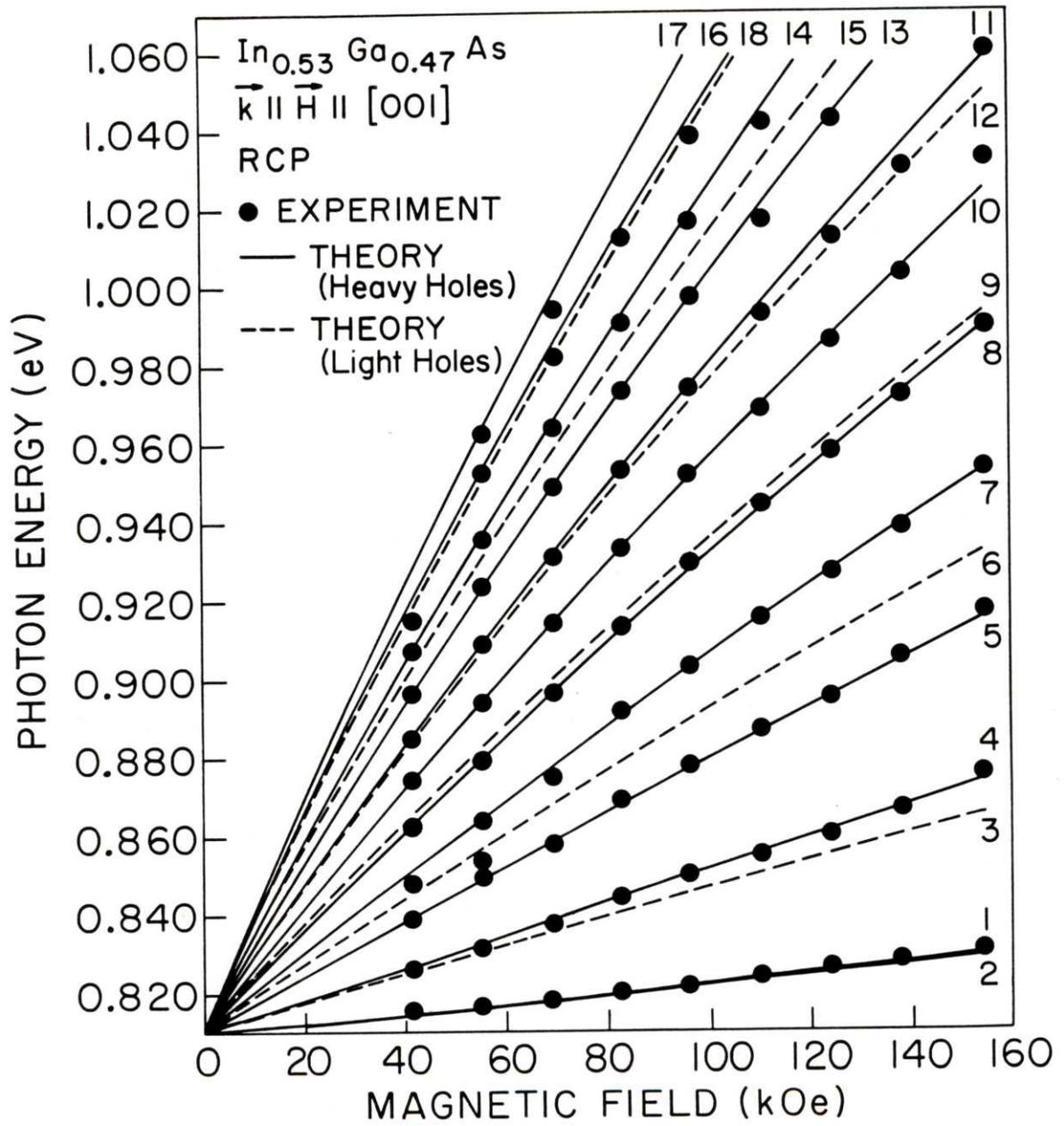
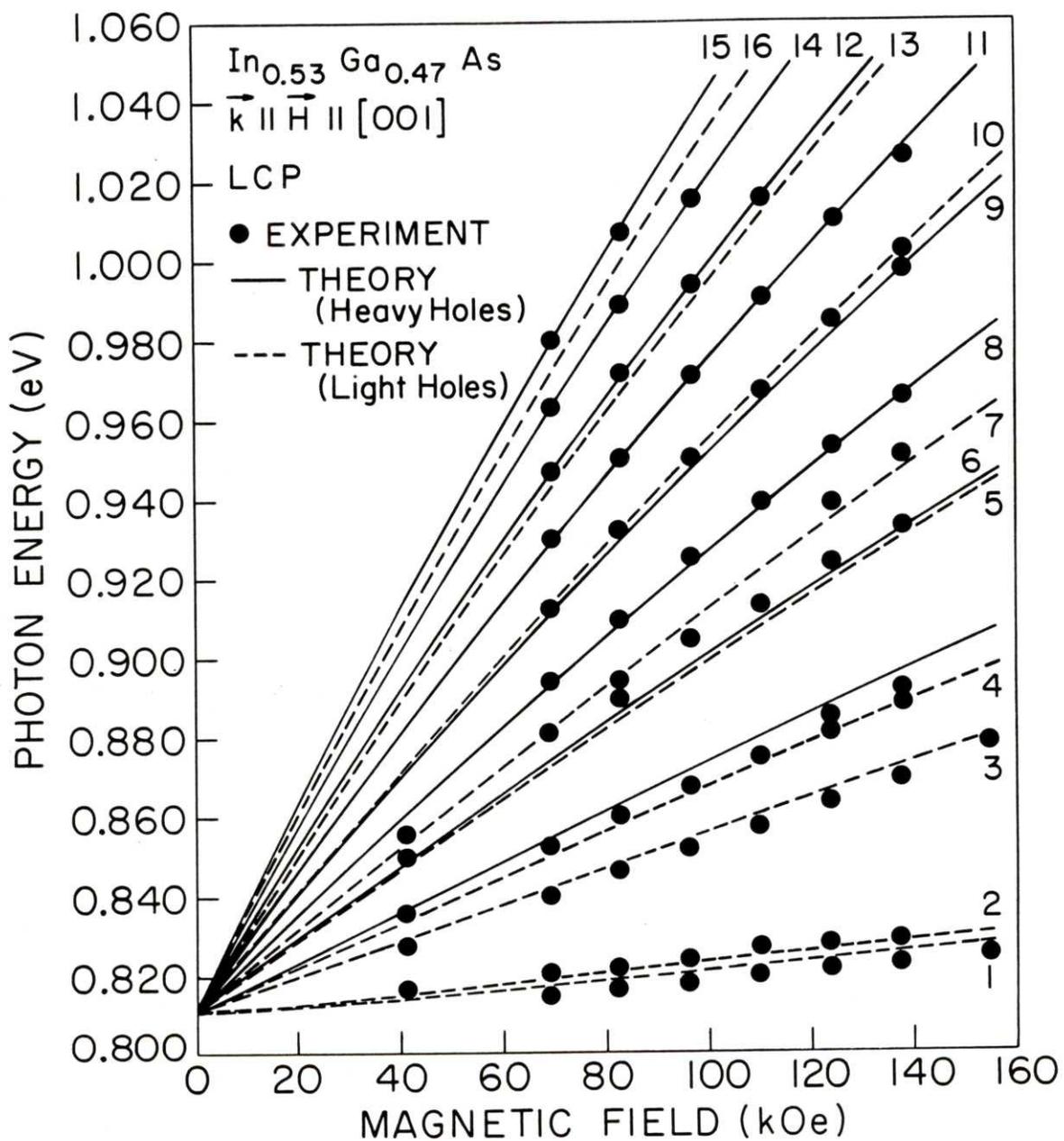


FIGURE IV-6 Point plot and fan chart (photon energy vs. magnetic field) for the interband transitions in the Faraday configuration ( $\vec{k} \parallel \vec{H}$ ) with LCP polarized light for the sample T9-50. The calculated transition lines are labeled according to Table IV-5. The unnumbered line corresponds to the two close-lying transitions  $a^-(1)a^c(2)$  and  $b^-(1)b^c(2)$ .



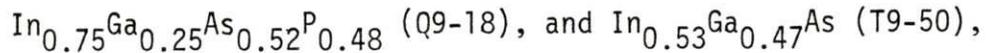
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CHAPTER VCONCLUSIONA. Summary

This work represents an account of the first interband magneto-optical investigations in members of the  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  semi-conducting alloy family which are important materials both technologically and from the point of view of the III-V semiconductor physics. In this thesis we have included our results of interband magneto-absorption for two samples:



both grown by liquid phase epitaxy on InP substrates of (100) orientation at M.I.T. Lincoln Laboratory. The experiments were carried out at M.I.T. Francis Bitter National Magnet Laboratory using high field Bitter magnets. Magnetoabsorption spectra were obtained, at near liquid helium temperatures, for several field values up to 155 kOe sweeping the wavelength of monochromatic infrared light, in both the Voigt configuration ( $\vec{k} \perp \vec{H}$ ) with  $\vec{E} \parallel \vec{H}$  and  $\vec{E} \perp \vec{H}$  polarization, as well as in the Faraday configuration ( $\vec{k} \parallel \vec{H}$ ) with right and left circular polarization. The structure in the spectra was attributed to optical transitions from the heavy and lighthole magnetic sub-bands to the conduction sub-bands and the transition energies obtained from the experimental spectra were used to form the basis of electronic

band analysis in the context of the quasi-Ge coupled band formalism. This analysis involves explicitly the conduction band, the heavy hole, the light hole, and the spin-orbit split-off valence bands of the fundamental edge, and treats the other bands as perturbations whose effect appears as adjustable coefficients in the quasi-Ge  $8 \times 8$   $\vec{k} \cdot \vec{p}$  Hamiltonian. This analysis was attempted to identify and fit the experimental data to the interband magneto-optical transitions. In the analysis we included an approximate exciton correction, which is small. This analysis was carried out to determine band parameters, which would best fit the interband measurements carried out in this work, consistent with physical considerations. A range of acceptable values for the band parameters was thus obtained. The quasi-Ge band parameters are  $E_g$ ,  $E_p$ ,  $\gamma_1$ ,  $\gamma_2$ ,  $\gamma_3$ ,  $\kappa$ ,  $F$ ,  $q$  and  $N_1$ , defined earlier. Our analysis shows that  $N_1$ , which is a small correction to the conduction band  $g$ -factor due to higher bands, does not affect our results. That is to say reasonable range of values for  $N_1$  leave our fits and our band parameters unchanged. A similar conclusion was reached regarding  $q$ . This means that these parameters could be set equal to zero. It was found that even for a relatively wide range of heavy hole mass  $m_-$  values, and a wide range of  $F$  (the higher bands' contribution to the conduction band mass  $m$ ), our best fits to the data would yield a very narrow range of values for the energy gap  $E_g$ , and the reduced effective masses  $\mu_+$  and  $\mu_-$  for the light (+) and heavy (-) hole to conduction band transitions. Similarly, a narrow range of values was obtained for

$\gamma_3 - \gamma_2$  when measurements were made with the magnetic field along more than one crystal axis. Since  $m_- \gg m_c$  the value of  $\mu_-$  is rather insensitive to  $m_-$ . Therefore, our magnetoabsorption measurements have been able to determine  $m_c$  within a narrow range. Hence, combining the result for  $\mu_+$  and  $m_c$ , the light hole mass  $m_+$  is also determined within a narrow range.

Our values for  $m_c$ , are in excellent agreement with intra-band measurements using cyclotron and magnetophonon resonance techniques. Furthermore, our results for  $\mu_+$ ,  $\mu_-$  and  $m_+$  are in excellent agreement with those obtained from optical pumping measurements recently reported.

The value of  $m_c$  cannot precisely determine the interband transition energy  $E_p$ . This is because of higher band contributions to the curvature of the  $\Gamma_6$  conduction band. This contribution can be as high as 20% compared to the contribution of the  $\Gamma_7$  and  $\Gamma_8$  valence bands. In fact our data accepts a rather wide range of  $F$  (between 0 and -3) resulting in an uncertainty in  $E_p$ . Values of  $E_p$  corresponding to  $F=0$  as well as those corresponding to the value obtained from linear interpolation among the binary constituents InAs, GaAs, and InP give good fits. The value of  $E_p$  can be narrowly determined provided the conduction band  $g$ -factor  $g_c$  is measured within a narrow range and  $E_g$  and  $\Delta$  are known, since  $N_1$ , representing the higher bands' contribution to  $g_c$ , is quite small. Recent preliminary measurements of  $g_c$  by optical pumping methods gives values for  $E_p$  close to the interpolated values.

The linear dependence of  $m_c$  upon  $y$ , which is strongly suggested by cyclotron and magnetophonon as well as our magnetoabsorption measurements, seems to suggest that the  $E_p$  values as a function of alloy composition  $y$  should show a small bowing downwards away from linearity. This point needs to be investigated further, and accurate  $g_c$  measurements will be useful in this regard.

Finally, if the exciton corrections are ignored the parameters deduced from the analysis would be affected by about 2% or less.

In summary, interband magneto-optical studies offer a relatively simple, and effective method for obtaining accurate measurements of a number of band parameters. These measurements do not require high concentration of conduction electrons and therefore give band parameters for  $\vec{k}=0$ . This is in contrast with some intra-band methods, such as Shubnikov-de Haas which require high electron concentration which then necessitates complicated corrections to the measured data.

#### B. Suggestions for Future Studies

In what follows, we give some suggestions for further experimental studies in the InGaAsP semiconducting alloy family.

1) Electroreflectance measurement of transitions from  $\Gamma_7$  as well as  $\Gamma_8$  bands to the  $\Gamma_6$  bands of the fundamental gap using

room temperature magnetoelectroreflectance or Schottky-Barrier magnetoelectroreflectance at low temperature.

- 2) Above studies using Stress-modulated magnetoreflexion.
- 3) Cyclotron resonance measurement of hole masses.
- 4) Accurate measurement of  $E_p$  by measuring  $g_c$  accurately using optical pumping methods which is already being carried out by others.
- 5) Interband magneto-optical studies in other members of this alloy family.
- 6) Study of the effect of lattice mismatch on the band parameters.

APPENDIX AELECTROREFLECTANCE OF InGaAsP/InP EPITAXIAL ALLOYS

Electroreflectance (ER) is a very sensitive technique for measuring the fundamental energy gap  $E_0$ , and the corresponding spin-orbit split-off band energy  $E_0 + \Delta_0$ , as well as higher energy critical points such as  $E_1$ ,  $E_1 + \Delta_1$ ,  $E'_0$ ,  $E'_0 + \Delta'_0$ , even at room temperature.<sup>1-3</sup> Recently the ER technique has been successfully applied to a member of the InGaAsP family to measure  $E_0$  and  $E_0 + \Delta_0$  at low temperature using Schottky barriers.<sup>4</sup> More recently, the electrolyte electroreflectance technique has been used to measure  $E_0$ ,  $E_0 + \Delta_0$ , and higher energy critical points.<sup>5,6</sup> In this report we present results of electroreflectance measurements in four different samples of InGaAsP and one sample of InP using the electrolyte technique.<sup>1,2</sup> The characteristics of the samples used in this study are summarized in Table A-1. The samples LPE - 91, LPE - 92, and LPE - 93 were provided by Dr. Zong-Long Liao of M.I.T. Lincoln Laboratory. These epitaxial samples were grown from the same melt composition at different growth temperatures (640.2°C, 628.6°C, and 630.85°C respectively), to give various lattice mismatches as in Table A-1.

The electroreflectance method as shown in the present study is sufficiently sensitive to detect slight variations in the energy gap  $E_0$  of the samples.

The samples were immersed in a sample cell containing a dilute electrolyte with a quartz window at the bottom making a small angle with the surface of the samples to separate out the unwanted reflection from the window. One electrode was soldered to the back of the sample. The edges and the back of the sample were covered with black wax for electric insulation from the electrolyte. A piece of platinum wire with one end immersed in the electrolyte made up the second electrode. A modulating voltage with square wave form at 85 Hz was applied between the two electrodes with or without the dc bias. With the resistivity of the electrolyte negligibly low this voltage drop occurs almost entirely in the narrow semiconductor-electrolyte interface, thus creating a high electric field on the surface of the semiconductor, normal to this surface. In addition to the external voltage, there is a built-in internal voltage at this interface of order of a few volts. The electrolyte used in case of the first three samples in Table A-1 was a 0.002 molar solution of KOH in deionized H<sub>2</sub>O. for the other two samples a very dilute solution of HF in deionized H<sub>2</sub>O (1-2 drop in 0.5 litre of H<sub>2</sub>O) was used. The optical setup is essentially similar to that described in Chapter III except for the following: (1) A single pass monochromator was used, (2) for the InP and Q9-77B sample we used a Bausch and Lomb grating with 640 lines/mm blazed for 1.4  $\mu\text{m}$  (blaze angle  $\theta_B=26^\circ 45'$ ) and for the LPE-91 through LPE-93 samples the grating had 300 lines/mm blazed for 1.0  $\mu\text{m}$  ( $\theta_B=8^\circ 38'$ ), (3) no dry air was used, and (4) the

incident light was not chopped. Light from the tungsten lamp was passed through the grating monochromator and filters, and was focused on the sample going through the quartz bottom window and the electrolyte. The light reflected from the sample was then focused on a room temperature PbS detector. Due to electric field modulation, the reflected signal had a modulated component,  $\Delta R$ . The modulated signal from the PbS detector,  $\Delta R$ , was detected by a lock-in amplifier locked to a reference signal synchronous with modulated voltage applied to the sample. The wavelength  $\lambda$  was swept and  $\Delta R$  vs.  $\lambda$  was stored on paper tape for computer analysis. For each sweep the conventional reflection spectrum,  $R$  vs.  $\lambda$ , was also obtained with a chopper and lock-in amplifier.  $\Delta R/R$  spectra were calculated numerically, and plotted vs. photon energy. Figures A-1 through A-3 show some of the electroreflectance spectra obtained in this study.

The intensities and energies of the observed peaks in the ER spectra are summarized in Table A-2. The values for  $E_0$  and  $E_0 + \Delta_0$  are calculated from our tabulated data using the three parameter method of Aspnes and Rowe,<sup>7</sup> although we realize that this method applies only to the low field regime for centrosymmetric crystals, or for certain polarizations and crystal surfaces (see Refs. 3, and 8-11) in case of zinc-blend type crystals. As is apparent from our spectra, one can see the onset of Franz-Keldysh oscillations which appear in the high-field regime.<sup>3</sup> The appearance of Franz-Keldysh oscillations as well as the large

magnitude of  $\Delta R/R$  even for peak-to-peak voltage,  $V_{pp}$ , of only 0.08 V is remarkable and shows that these quaternary samples possess relatively high electron mobility, compared to those in Refs. 5 and 16. Another feature of the spectra is the following. As shown for example for sample LPE-91 in Table A-2, the positions of A and B peaks remain constant within 1 meV and that of A' and B' peaks within 5 meV, when  $V_{pp}$  are varied from 0.08 to 2.0 volts. However, the intensity of the peaks do not scale linearly with  $V_{pp}$ . Here A and B refer to the largest peaks (corresponding to  $E_0$ ) with A having the lower energy,  $E_A < E_B$ . Similarly A' and B' refer to the  $E_0 + \Delta_0$  edge with  $E_{A'} < E_{B'}$ , do not scale linearly with  $V_{p-p}$ . The spectra, however, seem to shift with the applied dc voltage. The piezoreflectance contribution which could be present in our case (see Refs. 8-11) is estimated to introduce only a small correction to the spectra. This point, however, needs to be investigated in the future using the polarization dependence of this contribution. One point of uncertainty is the effect of the built-in potential on shifting the values of  $E_0$  and  $E_0 + \Delta_0$ , which could depend on the electrolyte used. However, this dependence on the dc voltage is expected to be small. For instance, from lines 7-9 in Table A-2, it is apparent that a change of 1.16 V in the dc bias shifts the A and B peaks only 10 meV, and the  $E_0$  value calculated by the three parameter method of Aspnes and Rowe<sup>7</sup> shows only a 4 meV shift and  $E_0 + \Delta_0$ , a 19 meV shift. This point needs further investigation. Finally, the

small variation in the lattice mismatch induces remarkable changes in the spectra, in terms of peak positions and line widths, as seen in Figure A-3. The new small peaks between the two largest peaks in the LPE - 92 spectra may be due to the strains induced by the relatively large lattice mismatch.

In conclusion, we have shown our first results of electrolyte electroreflectance of some members of the InGaAsP family with some of the samples purposely lattice mismatched to the InP substrates. Spectra show quantitative as well as qualitative differences. We believe electroreflectance offers a very sensitive tool in observing such changes. We suggest that further investigations especially with polarized light and as a function of dc bias could facilitate further understanding of the spectra. Finally, it is noted that the spin-orbit split-off edge is observable with the aid of electroreflectance method even at room temperature. Therefore, magneto-optical measurement of the spin-orbit split-off to conduction band transitions in the quaternary alloys should be possible, using electrolyte method at room temperature, as reported for Ge, GaSb, InSb, and InAs.<sup>13,14</sup>

TABLE A-1 Characteristics of the epitaxial  $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$  samples grown on InP substrates used in the present electroreflectance studies.

Sample	x	y	$\Delta a/a^*$	$E_0$ (eV)
InP**	0	0	-	1.34 §
Q9-77B	0.23	0.52	$\leq 6 \times 10^{-4}$	1.0 §§
LPE-91	(0.17)+	(0.4)+	-0.143%	1.08
LPE-92	(0.17)	(0.4)	+0.205%	"
LPE-93	(0.17)	(0.4)	0.13%	"

\* Lattice constant mismatch of epitaxial layers relative to InP substrates.

\*\*Bulk sample.

§ Reference 1 of this Appendix.

§§ Estimated from Reference 15 of this Appendix.

+ Values in parenthesis are those given in Table 1, line 1 of Reference 12 for quaternary grown from the same melt composition at a different temperature resulting in  $\frac{\Delta a}{a} \leq 0.03$ . This melt composition consisted of the following atom fraction percentages: In(95.77%), Ga(0.35%), As(3.54%) and P(0.34%).

TABLE A-2 Summary of the electroreflectance measurements. External V is measured from the platinum electrode to the sample electrode.

Line Figure	Sample	$\frac{\Delta a}{a}$ %	electrolyte	External dc	V(volts) pp	$E_A$ (eV) $10^6(\Delta R/R)$	$E_B$ (eV) $10^6(\Delta R/R)$	$E_O$ (eV)*	$E_A'$ (eV) $10^6(\Delta R/R)$	$E_B'$ (eV) $10^6(\Delta R/R)$	$E_O + \Delta_O$ (eV)*	$\Delta_O$ (eV)*
1 A-1	InP	--	KCl/H <sub>2</sub> O	-2.2	3.0	1.337 -44814	1.356 24492	1.342	1.439 6196	1.471 180	1.442	0.100
2 A-2	Q9-77B	--	KCl/H <sub>2</sub> O	1.0	2.0	0.978 -13412	0.999 10285	0.986	1.235 -166	1.269 579	1.264	0.278
3	LPE-91-0.143		KCl/H <sub>2</sub> O	0.0	0.08	1.096 -2598	1.115 1285	1.101	1.305 -145	1.343 37	1.310	0.209
4 A-3	LPE-91-0.143		KCl/H <sub>2</sub> O	0.0	0.4	1.096 -9675	1.115 4733	1.101	1.309 -544	1.348 44	1.310	0.209
5	LPE-91-0.143		KCl/H <sub>2</sub> O	0.0	2.0	1.094 -17934	1.114 9623	1.100	1.309 -955.5	1.340 47.5	1.310	0.210
6 A-3	LPE-92 0.203		HF/H <sub>2</sub> O	0.0	0.4	1.037 -9043	1.081 11548	1.063	1.269 -676	1.314 983	1.296	0.233
7	LPE-93 0.13		HF/H <sub>2</sub> O	0.0	0.4	1.059 -31337	1.096 9971	1.065	1.286 -2475	1.334 1468	1.302	0.237
8	LPE-93 0.13		HF/H <sub>2</sub> O	0.56	0.4	1.063 -28477	1.090 6821	1.066	1.230 342	1.291 -2350	1.290	0.224
9	LPE-93 0.13		HF/H <sub>2</sub> O	0.6	0.4	1.054 -23976	1.098 7997	1.062	1.284 -1468	1.332 1209	1.305	0.243
10 A-3	LPE-93 0.13		HF/H <sub>2</sub> O	0.0	0.4	1.054 -25116	1.098 10183	1.064	1.282 -1863	1.329 1559	1.303	0.239

\*Based on the three-point method of Reference 7.

FIGURE A-1 Electrolyte electroreflectance spectrum of the InP bulk sample from (100) surface. In this and all of the other measurements the external applied voltage was measured as the voltage drop from the platinum electrode to the sample electrode measured externally. The two larger peaks A and B ( $E_A < E_B$ ) correspond to the fundamental edge, and the A' and B' ( $E_{A'} < E_{B'}$ ) peaks, to the corresponding spin-orbit split-off edge.

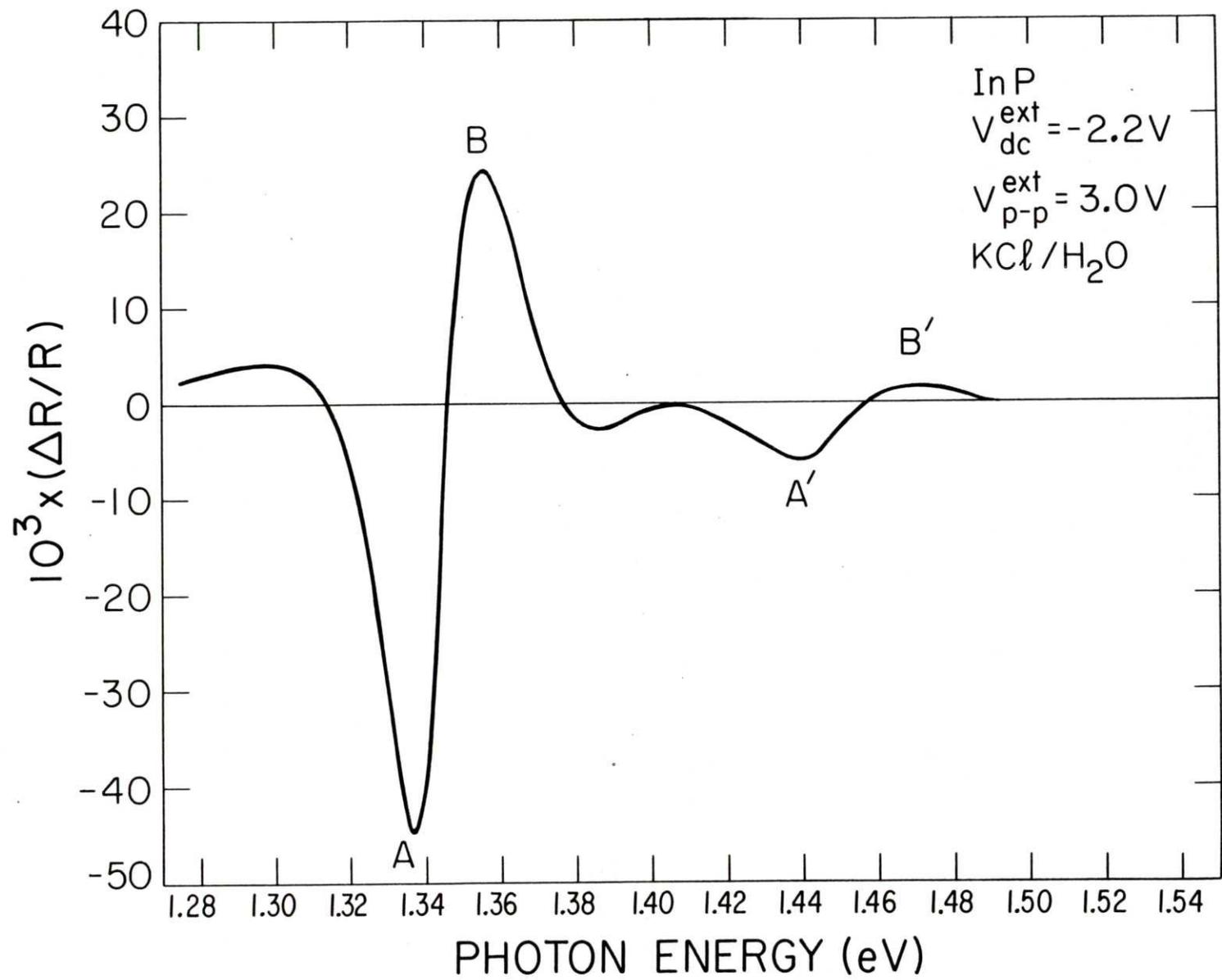


FIGURE A-2 Electrolyte electroreflectance of spectrum of the quaternary sample Q9-77B from (100) surface. Note the onset of Franz-Keldysh oscillations.

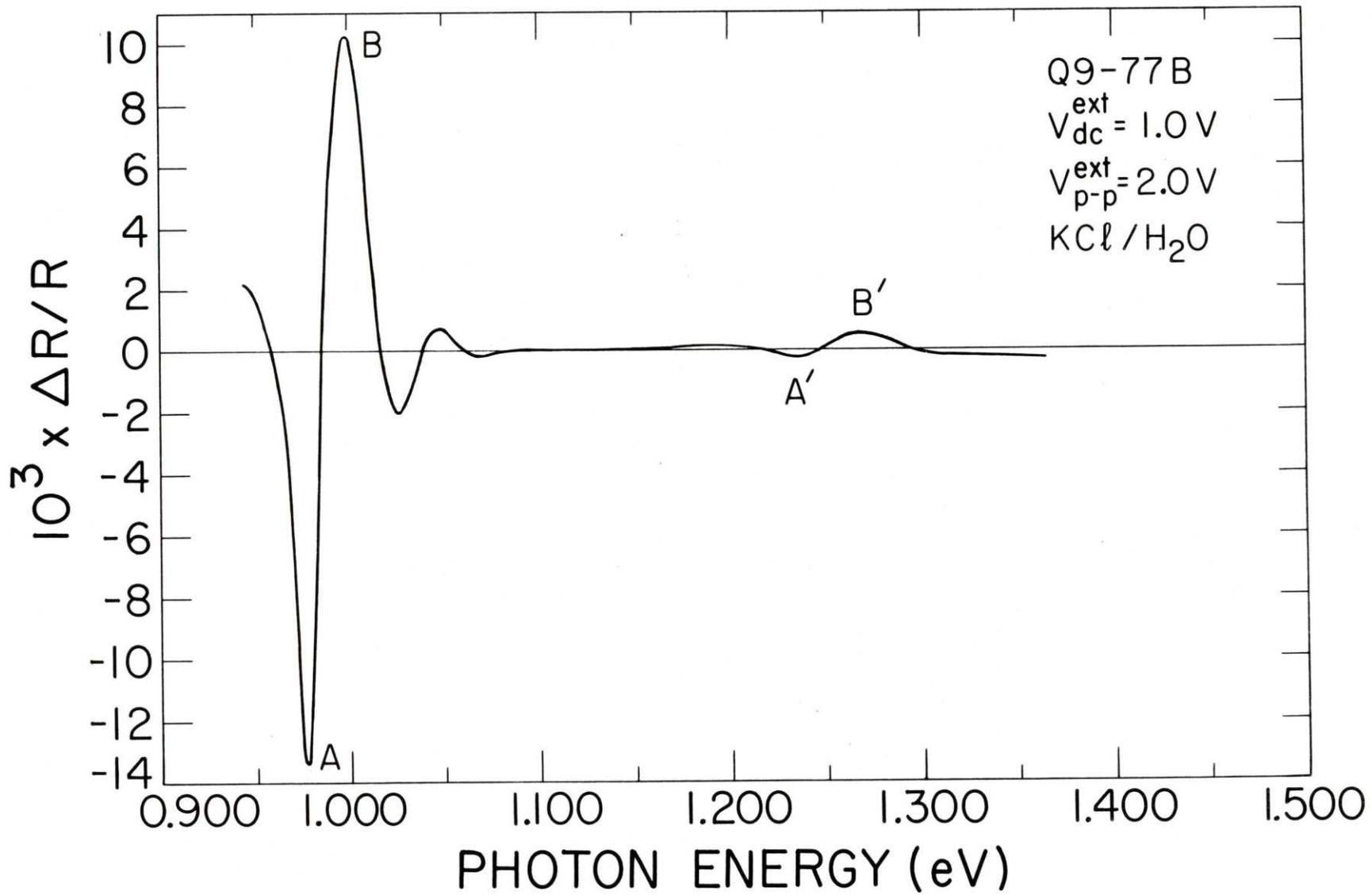
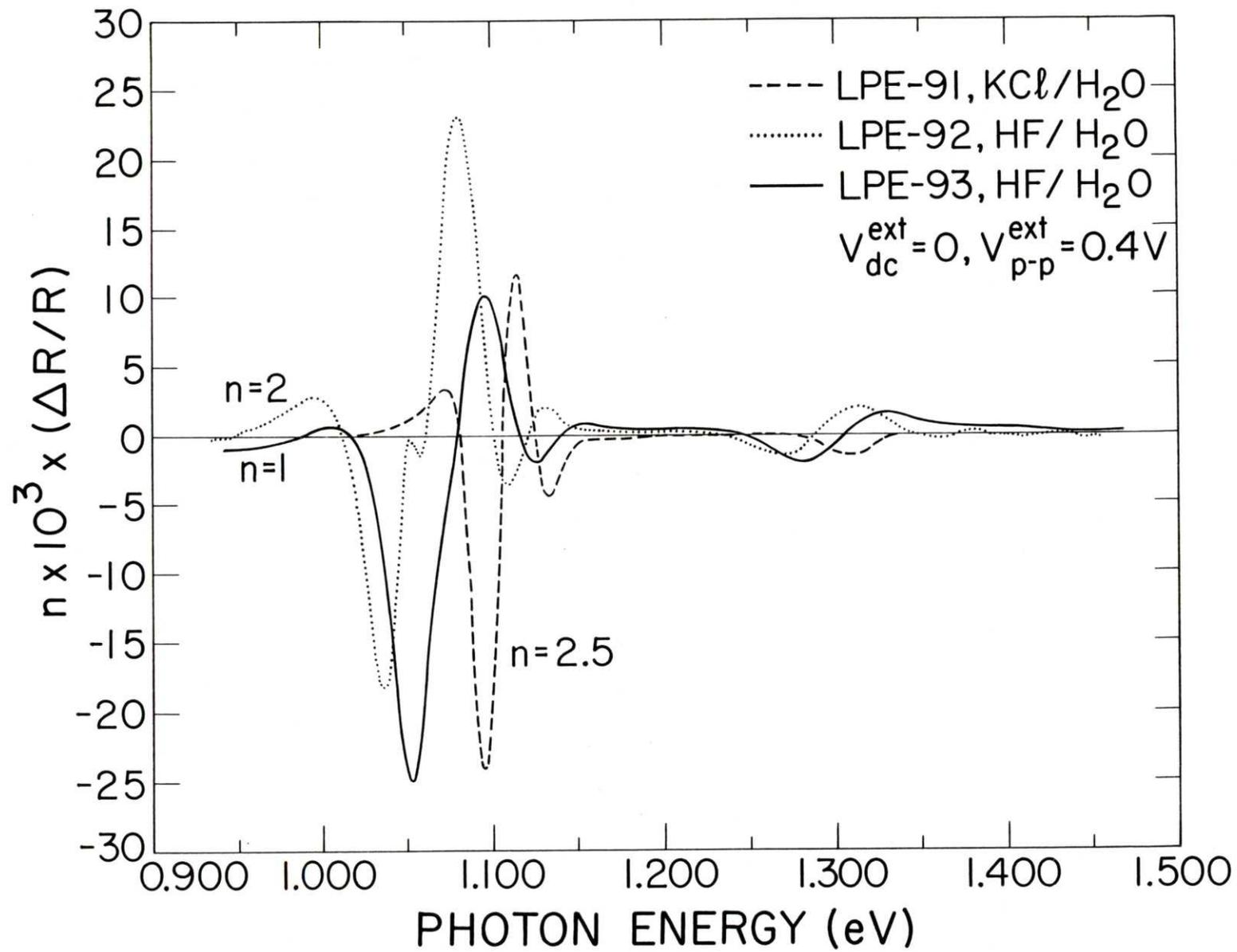


FIGURE A-3 Electrolyte electroreflectance spectrum of the three quaternary samples LPE-91, LPE-92, and LPE-93. Note the qualitative differences as well as the change in peak positions and linewidths among the three samples. The two small peaks between the two large ones in the LPE-92 spectrum may be caused by the strains due to the relatively large lattice mismatch with the substrate.



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## APPENDIX B

THE  $\vec{k} \cdot \vec{p}$  PARAMETERS AND ESTIMATIONS

The  $\vec{k} \cdot \vec{p}$  parameters of Table II-2 will be given here in terms of sums over intermediate states when applicable. Some of these parameters are related to those introduced by Kane<sup>1</sup> who used the single group representations of  $T_d$  instead of the double group representation used by Weiler.<sup>2</sup>

$$1) \quad P \equiv -i(\hbar/m) \langle S | p_x | X \rangle \quad (\text{Ref. 1}) \quad (\text{B-1})$$

2)  $C$  is allowed by the spin-orbit interaction and is defined by Dresselhaus,<sup>3</sup>

$$C \equiv \frac{\hbar^2}{2\sqrt{3} m^2 c^2} \sum_{\Gamma'_i = \Gamma'_4, \Gamma'_5} \frac{\langle Y \uparrow | H_{so} | \Gamma'_i \uparrow \rangle \langle \Gamma'_i \uparrow | p_y | Z \uparrow \rangle}{E_0 - E(\Gamma'_i)}$$

Where  $E_0$  is the valence band energy at  $\vec{k}=0$ . The  $P$  and  $C$  are parameters in the single group representation of  $T_d$ . In the double group representation, additional parameters  $P'$  and  $C'$  are obtained. These new parameters are expected to be very close to the unprimed ones.

3) The parameters  $\gamma_1, \gamma_2, \gamma_3, \kappa$  are linear combinations of the Kane parameters  $A_K, B_K, C_K,$  and  $D_K$ :

$$\gamma_1 = -\frac{2}{3}(A_K + B_K + 2C_K + 2D_K) - 1 \quad (\text{B-3a})$$

$$\gamma_2 = -\frac{1}{3}(A_K + B_K - C_K - D_K) \quad (\text{B-3b})$$

$$\gamma_3 = -\frac{1}{3}(A_K - \frac{1}{2} B_K + C_K - D_K) \quad (\text{B-3c})$$

$$\kappa = -\frac{1}{3}(A_K - \frac{1}{2} B_K - C_K + D_K) - \frac{1}{3} \quad (\text{B-3d})$$

The Kane parameters are defined in terms of matrix elements of  $\vec{p}$  among the  $\vec{k}=0$  states belonging to the single-group representation of  $T_d$ ,

$$\begin{aligned} A_K &\equiv \frac{1}{m} \sum_{\Gamma_1'} \frac{|\langle X | p_x | \Gamma_1' \rangle|^2}{E_c - E(\Gamma_1')}, & B_K &\equiv \frac{1}{m} \sum_{\Gamma_3'} \frac{|\langle X | p_x | \Gamma_3' \rangle|^2}{E_0 - E(\Gamma_3')} \\ C_K &\equiv \frac{1}{m} \sum_{\Gamma_4'} \frac{|\langle X | p_y | \Gamma_4' \rangle|^2}{E_0 - E(\Gamma_4')}, & D_K &\equiv \frac{1}{m} \sum_{\Gamma_5'} \frac{|\langle X | p_y | \Gamma_5' \rangle|^2}{E_0 - E(\Gamma_5')} \end{aligned} \quad (\text{B-4})$$

where  $E_0$  is the  $\vec{k}=0$  energy of the valence band ( $E_v$ ). The other Kane parameters are

$$F = \frac{1}{m} \sum_{\Gamma_4'} \frac{\langle S | p_x | \Gamma_4' \rangle}{E_0 - E(\Gamma_4')} \quad (\text{B-5})$$

where in Eq.(B-4)  $E_0$  is the conduction band energy at  $\vec{k}=0$ , (i.e.,  $E_c$ ).

$$G = \frac{1}{m} \sum_{\Gamma_4'} \frac{\langle S | p_x | \Gamma_4' \rangle \langle \Gamma_4' | p_x | Z \rangle}{E_0 - E(\Gamma_4')} \quad (\text{B-6})$$

where  $E_0$  is an average of  $E_c$  and  $E_v$ . Actually for  $E(\Gamma_4') \gg E_g \equiv (E_c - E_v)$ ,  $G$  would be insensitive to whether one uses  $E_c$  or  $E_v$ .

4) When the spin-orbit splitting of the higher  $\Gamma_4$  bands is included (i.e.,  $\Gamma_4' \rightarrow \Gamma_8', \Gamma_7'$ ) another four parameters are obtained:<sup>2</sup>

$$q = \frac{8}{27} \frac{i}{m} \sum_{\Gamma_8'} \frac{\langle \psi_{3/2}^8 | p_x | \Gamma_8' \rangle \langle \Gamma_8' | p_y | \psi_{3/2}^8 \rangle}{E_v - E(\Gamma_8')} \quad (\text{B-7})$$

$$N_1 = -\frac{i}{m} \sum_{\Gamma_8'} \frac{\langle \psi_{1/2}^6 | p_x | \Gamma_8' \rangle \langle \Gamma_8' | p_y | \psi_{1/2}^6 \rangle}{E_c - E(\Gamma_8')} \quad (\text{B-8})$$

$$N_2 = \frac{1}{m} \sum_{\Gamma_8'} \frac{\langle \psi_{1/2}^6 | p_x | \Gamma_8' \rangle \langle \Gamma_8' | p_x | \psi_{-3/2}^8 \rangle}{E_o - E(\Gamma_8')} \quad (\text{B-9})$$

$$N_3 = -\frac{i}{m} \sum_{\Gamma_8'} \frac{\langle \psi_{1/2}^6 | p_x | \Gamma_8' \rangle \langle \Gamma_8' | p_y | \psi_{-3/2}^8 \rangle}{E_o - E(\Gamma_8')} \quad (\text{B-10})$$

In the single group approximation  $N_1$  can be expressed as

$$N_1 \approx \frac{1}{3m} \sum_{\Gamma_4'} \frac{|\langle S | p_x | \Gamma_4' \rangle|^2}{[E_c - E(\Gamma_4')]^2} \frac{\Delta_o'}{[E_c - E(\Gamma_4')]} \quad (\text{B-11})$$

where

$$\Delta_o' = E(\Gamma_8^C) - E(\Gamma_7^C) \quad (\text{B-12})$$

as shown in Figure II-1. The higher-band energies which appear throughout this Appendix are those for  $\vec{k}=0$ .

Considering the leading term explicitly Eq.(B-11) can be written as<sup>4</sup>

$$N_1 \approx \frac{1}{3m} |\langle S | p_x | \Gamma_4' \rangle|^2 \left( \frac{E(\Gamma_8^C) - E(\Gamma_7^C)}{[E_c - E(\Gamma_7^C)][E_c - E(\Gamma_8^C)]} \right) + C' \quad (B-13)$$

where  $\Gamma_8^C$  and  $\Gamma_7^C$  are the next higher energy bands beyond the four-bands which have been considered explicitly in the  $8 \times 8 \vec{k} \cdot \vec{p}$  analysis and

$$C' = \frac{1}{3m} \sum_{\Gamma_4''} \frac{|\langle S | p_x | \Gamma_4' \rangle|^2 \cdot \Delta_0''}{[E_c - E(\Gamma_4'')]^2} \quad (B-14)$$

is the contribution from all other intermediate states. We define

$$E_p' \equiv (2/m) |\langle S | p_x | \Gamma_4' \rangle|^2 \equiv P'^2 \quad (B-15)$$

Similarly for  $q$ , in the single-group approximation, one obtains

$$q \approx \frac{4}{9m} \sum_{\Gamma_4'} \frac{|\langle x | p_y | \Gamma_4' \rangle|^2 \Delta_0'}{[E_0 - E(\Gamma_4')]^2} \quad (B-16)$$

which yields

$$q \approx -\frac{4}{9} \frac{\Delta_0'}{E(\Gamma_4^C) - E_V} C_K \quad (B-17)$$

in agreement with the result of Hensel and Suzuki.<sup>5</sup> Eqs. (B-11) and (B-5) give

$$N_1 \approx \frac{1}{3} \frac{\Delta'_0}{E(\Gamma_4^C) - E_C} F \quad (\text{B-18})$$

In Eqs. (B-17) and (B-18) for  $E(\Gamma_4^C)$  we can use  $\Gamma_8^C$  or  $\Gamma_7^C$ , since  $\Delta'_0 \ll \Gamma_7^C \sim \Gamma_8^C$ .

We take Eq.(B-17) further. From Eqs.(B-3) it is seen that

$$C_K = D_K + \frac{1}{2}(3\kappa - 3\gamma_3 + 1) \quad (\text{B-19})$$

the parameter  $D_K$  is estimated to be nearly zero in most of the literature which gives

$$-\frac{1}{4}\gamma_1 + \frac{1}{2}\gamma_2 + \frac{3}{4}\gamma_3 - \frac{3}{4}\kappa - \frac{1}{2} = D_K = 0 \quad (\text{B-20})$$

and

$$C_K = \frac{1}{2}(3\kappa - 3\gamma_3 + 1) \quad (\text{B-21})$$

Hence, a knowledge of the higher band energies  $E(\Gamma_8^C)$  and  $E(\Gamma_7^C)$  helps to reduce the number of parameters by relating  $q$  and  $N_1$  to the rest of  $\vec{k} \cdot \vec{p}$  parameters through Eqs.(B-18) and (B-21).

### Estimation of $N_1$

Hermann and Weisbuch<sup>4</sup> have also considered explicitly one set of higher bands namely  $\Gamma_4^C$  (which in their notation is called  $\Gamma_5^C$ ) which consist of the doubly degenerate  $\Gamma_8^C$  and spin orbit split-off  $\Gamma_7^C$  (see Figure II-2). There are two typographical errors in their paper: In Eq.(4)  $P^2$  should read  $-P^2$  and in Eq.(6)  $A$  multiplies everything to its right and not just the first term. Using their expressions we get

$$F = -\frac{1}{6} P'^2 \left( \frac{2}{E(\Gamma_8^C) - E_g} + \frac{1}{E(\Gamma_7^C) - E_g} \right) + \frac{1}{2} C \quad (\text{B-22})$$

$$N_1 = -\frac{1}{6} P'^2 \left( \frac{-1}{E(\Gamma_8^C) - E_g} + \frac{1}{E(\Gamma_7^C) - E_g} \right) + \frac{1}{2} C' \quad (\text{B-23})$$

where  $P'^2$  is the interband transition energy proportional to the square of momentum matrix element,  $C$  and  $C'$  come from other higher bands not included explicitly with  $C \approx -2$  or perhaps  $-1$  and  $C' \approx -0.02$ . One observation is that  $N_1 \ll F < 0$ . Table B-2 summarizes some of the values useful for Eqs.(B-22) and (B-23). These equations give  $N_1$  in terms of  $F$ :

$$N_1 = \frac{\Delta'_0}{2[E(\Gamma_7^C) - E_g] + [E(\Gamma_8^C) - E_g]} \left( F - \frac{C}{2} \right) + C' \quad (\text{B-24})$$

which is close enough to Eq.(B-18). Using  $E_g = 0.813 \text{ eV}$  for the ternary and  $E_g = 1.065 \text{ eV}$  for the quaternary and using interpolated values from

TABLE B-1 Some of the band parameters for InAs, GaAs, InP as well as values obtained from linear interpolation for the ternary and the quaternary samples (refer to Figure II-1).

	<sup>a</sup> InAs	<sup>a</sup> GaAs	<sup>b</sup> In <sub>0.53</sub> Ga <sub>0.47</sub> As	<sup>a</sup> InP	<sup>b</sup> In <sub>0.75</sub> Ga <sub>0.25</sub> As <sub>0.52</sub> P <sub>0.48</sub>	
E <sub>g</sub> (eV)	0.42	1.519	(0.937)	1.423	(1.70)	
Δ(eV)	0.38	0.34	(0.36) 0.35±0.01 <sup>d</sup>	0.108 <sup>c</sup>	(0.24) 0.23 <sup>e</sup>	
*E' <sub>0</sub> (eV)	4.60	4.659	(4.63)	4.79	(4.71)	
**E' <sub>0</sub> +Δ' <sub>0</sub> (eV)	4.44	4.488	(4.46)	4.72	(4.62)	
Δ' <sub>0</sub> (eV)	0.16	0.171	(0.165)	0.07	(0.12)	
m <sub>c</sub> /m	0.0230	0.0667		0.0803		
g <sub>c</sub> (exp'tal)	-14.8	-0.44	-4.2±25% <sup>f</sup>	1.26		
P <sup>2</sup> ≡E <sub>p</sub> (eV)	22.2± 0.5	28.9± 0.9	(25.35)	20.7± 1.5	(23.1)	
P <sup>2</sup> ≡E <sub>p</sub> (eV)	$\begin{cases} C=-2 \\ C=-1 \end{cases}$	0.2	6	(2.8)	2.1	(2.5)
		4	9	(6.4)	6	(6)
F	-1±1	-1.9± 0.5	(-1.4±0.8)	-0.9±1	(-1.2±0.9)	

<sup>a</sup>Taken from Ref. 4, unless otherwise noted.

<sup>b</sup>Values in parantheses are from linear interpolations.

<sup>c</sup>After Ref. 6.

<sup>d</sup>After Ref. 7.

<sup>e</sup>Estimated from Ref. 7.

<sup>f</sup>After Ref. 9.

$$*E'_0 \equiv E(\Gamma_7^C) - E(\Gamma_7^V)$$

$$**E'_0 + \Delta'_0 \equiv E(\Gamma_8^C) - E(\Gamma_7^V)$$

Table B-1 we get

TABLE B-2

		C=-2, C'=-0.02	C=-1, C'=0.02	Eq.(B-18)
T9-50	$N_1 \approx$	(0.014)F - 0.034	(0.014)F - 0.027	0.014 F
Q9-18	$N_1 \approx$	(0.011)F - 0.031	0.011 F - 0.026	0.011 F

This shows that  $N_1$ , the higher band contribution to  $g_c$ , is much smaller than F, the higher band contribution to  $m_c$ , as pointed out in Ref.4. For physically reasonable values of F,  $N_1$  is seen to be very small (see Table B-1) so that it can be neglected in Eq.(3-18).

Thus

$$g_c = 2 \left[ 1 - \frac{E_p}{3} \frac{\Delta}{E_g(E_g + \Delta)} \right] \quad (B-25)$$

Precise measurement of  $g_c$ , and  $E_g$  thus yields  $E_p$  ( $P^2$  in the notation of Ref.4) to a good precision. This value of  $E_p$  can then be used to obtain F using Eq.(2-17), since  $m_c$  can be determined very precisely using interband magnetoabsorption or cyclotron resonance. The effect of higher bands on  $m_c$  and  $g_c$  was considered for InSb earlier by Groves, in a similar fashion.<sup>8</sup>

Estimate of q

Using Eqs.(B-17) and (B-21) and Table B-1 we can estimate q:

$$q \approx -\frac{4}{3} \frac{\Delta'_0}{2E(\Gamma_7^C) + E(\Gamma_8^C)} C_K \quad (B-17)'$$

$$q \approx \frac{1}{2}(-3\kappa + 3\gamma_3 - 1) \times \begin{cases} (0.017) & \text{for T9-50} \\ (0.011) & \text{for Q9-18} \end{cases} \quad (B-26)$$

We can use Table B-2 and Eq.(B-26) as two constraint equations in our minimization routine (Ch.IV). It turns out that for the values of  $\kappa$ , and  $\gamma_3$  obtained from our minimization routine q is very small, just as  $N_1$  turns out to be. For typical values of q and  $N_1$  the effect of these parameters on our experimental spectra is negligible and they can be set equal to zero.

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APPENDIX C

NONPARABOLICITY OF THE CONDUCTION BAND

C. 1. Conduction Band Energies Up to  $H^2$  (or  $k^4$ )

In Chapter II, Eq.(2-52), we presented an expression for the energy of the conduction band up to  $k^4$ , which included F, the higher bands' contribution to  $m_c$ . This can be rewritten as

$$E_c = E_g + \left(\frac{m}{m_c}\right) \frac{\hbar^2 k^2}{2m} - \left(\frac{m}{m_c} - 1 - 2F\right) \left(\frac{m}{m_c} - 1\right) \left(\frac{3+4Q+Q^2}{3+5Q+Q^2}\right) \frac{1}{E_g} \left(\frac{\hbar^2 k^2}{2m}\right)^2 \quad (C-1)$$

where

$$Q \equiv (\Delta/E_g) \quad (C-2)$$

In a magnetic field, the average of a- and b-series energies for a given n is obtained when the following substitution is made in Eq.(C-1):

$$\left(\frac{\hbar^2 k^2}{2m}\right) \rightarrow \left(n + \frac{1}{2}\right) (2\mu_B H) \quad (C-3)$$

The result is

$$E_c(n) = E_g + \left(n + \frac{1}{2}\right)^2 \frac{\hbar^2 k^2}{2m} - \left(n + \frac{1}{2}\right)^2 (2\mu_B H)^2 \frac{1}{E_g} \times \left(\frac{m}{m_c} - 1 - 2F\right) \left(\frac{m}{m_c} - 1\right) \left(\frac{3+4Q+Q^2}{3+5Q+Q^2}\right) \quad (C-4)$$

Note that in the derivation of Eqs. (C-3) and (C-4) the assumption is

that  $\gamma_1 = -1$ ,  $\gamma_2 = \gamma_3 = 0$ ,  $\kappa = -\frac{1}{3}$ , as in Kane's model, which ignores the effect of higher bands. To obtain expression which allcwvalues for  $\gamma_1$ ,  $\gamma_2$ ,  $\gamma_3$  and  $\kappa$  other than the above, we can follow the treatment presented in Ref. 1. According to this presentation first the determinant equations for the eigenvalue problems of Eqs.(2-13), for the quasi-Ge model have been obtained [Eq.(102), Ref.1)]. The eigen-energies are then assumed to have a power series expansion in powers of  $(2\mu_B H)$ :

$$E_c = E_g + (2\mu_B H) E_1^c + (2\mu_B H)^2 E_2^c + \dots \quad (C-5)$$

One can then obtain

$$E_1^c = (n + \frac{1}{2}) \frac{m}{m_c} \pm \frac{1}{4} g_c \quad (C-6)$$

where + is for the a-series and - for the b-series. For the mean value of  $E_2^c$  for a and b series we have obtained

$$E_2^c = - (n + \frac{1}{2})^2 \cdot \frac{1}{E_g} \left( \frac{m}{m_c} - 1 - 2F \right) \{ Q_1 \left( \frac{m}{m_c} + \gamma_1 \right) + Q_2 (\gamma' + 3\gamma'') \} + \eta + \xi \quad (C-7)$$

$$\text{where } \begin{cases} Q_1 \equiv \frac{3+4Q+2Q^2}{3+5Q+2Q^2} \end{cases} \quad (C-8)$$

$$\begin{cases} Q_2 \equiv \frac{3+Q}{3+2Q} \end{cases} \quad (C-9)$$

and  $\eta$  and  $\xi$  are independent of  $n$ .

$$\eta = -\frac{1}{E_g} \left(\frac{m}{m_c} - 1 - 2F\right) \left\{ \frac{1}{4} [(1-Q_2) \left(\frac{m}{m_c} - 1 - 2F\right) - 1] \right\} \times \quad (C-10)$$

$$\times (2-Q_1-Q_2)$$

$$\xi = -\frac{1}{E_g} \left(\frac{m}{m_c} - 1 - 2F\right) \left\{ \frac{1}{2} Q_1 \gamma_1 + \frac{1}{4} Q_2 (2\gamma' - 3\gamma'') \right. \quad (C-11)$$

$$\left. - \frac{1}{4} (2Q_1 + Q_2) \kappa - \frac{1}{4} \frac{1}{1+Q} \right\}$$

$$E_c = \left(n + \frac{1}{2}\right) \left(\frac{m}{m_c}\right) (2\mu_B H) - \left(n + \frac{1}{2}\right)^2 \left(\frac{m}{m_c} - 1 - 2F\right) \times \quad (C-13)$$

$$\times \left\{ Q_1 \left(\frac{m}{m_c} + \gamma_1\right) + Q_2 (\gamma' + 3\gamma'') \right\} \frac{1}{E_g} (2\mu_B H)^2 + n + \xi$$

It turns out that the first term in Eq.(C-7) is much larger than  $\eta$  and for large  $n$  certainly much larger than both  $\eta$  and  $\xi$ .

Therefore, in Eq.(C-7) we can ignore  $\eta$  and  $\xi$  for large  $n$ . Thus the nonparabolicity of the conduction band up to  $k^4$  can be determined from Eq.(C-7) when the following substitution is made:

$$\left(n + \frac{1}{2}\right) (2\mu_B H) \rightarrow \frac{\hbar^2 k^2}{2m} \quad (C-14)$$

We then obtain

$$E_c = \left(\frac{m}{m_c}\right) \frac{\hbar^2 k^2}{2m} - \left(\frac{m}{m_c} - 1 - 2F\right) \left\{ Q_1 \left(\frac{m}{m_c} + \gamma_1\right) + Q_2 (\gamma' + 3\gamma'') \right\} \frac{1}{E_g} \left(\frac{\hbar^2 k^2}{2m}\right)^2 \quad (C-15)$$

or

$$E_c = E_0 \left(1 - \alpha \frac{E_0}{E_g}\right) \quad (C-16)$$

where

$$E_0 = \frac{\hbar^2 k^2}{2m_c} \quad (C-17)$$

and

$$\alpha \equiv \left(\frac{m_c}{m}\right)^2 \left(\frac{m}{m_c} - 1 - 2F\right) \{Q_1\left(\frac{m}{m_c} + \gamma_1\right) + Q_2(\gamma'_1 + 3\gamma''_1)\} \quad (C-18)$$

In the Kane model  $F=0$ ,  $\gamma_1 = -1$ ,  $\gamma'_1 = \gamma''_1 = 0$ , and one can recover expressions given for example by Vrethen<sup>2</sup> who found  $\alpha=0.83$  for GaAs. It is important to note that Eqs.(C-13) and (C-18) determine the nonparabolicity more accurately since Kane model is only an approximation.

## C. 2. Nonparabolicity of the Conduction Band and Interband Transitions

It is seen in the Figures of Chapter IV (especially those for the Voigt and the RCP polarization configurations), for a given magnetic field value, the spacing between adjacent transitions decreases as one goes higher in energy. This is a consequence of the nonparabolicity of the conduction band and can be seen from Eq.(C-13).

In the point plots for the Voigt and the RCP configurations we can assume that the minima come essentially from the heavy hole-to-conduction band transitions, and the nonparabolicity of the heavy hole band can be ignored (since it has a much heavier effective mass) consequently using Eqs.(2-23), (C-13) and (C-18) we have obtained the

following expression for the energy separation between two adjacent transitions for a given H where n is the conduction band quantum number:

$$E(n) - E(n-1) = \left(\frac{m}{m_c} + \frac{m}{m_-}\right)(2\mu_B H) - \left[\left(n + \frac{1}{2}\right) - \left(n - \frac{1}{2}\right)\right]^2 \alpha \frac{1}{E_g}(2\mu_B H) \left(\frac{m}{m_c}\right)^2 \quad (C-19)$$

$$\varepsilon(n) \equiv \frac{E(n) - E(n-1)}{2\mu_B H} = \left(\frac{m}{\mu_-}\right) - 2n\alpha \left(\frac{m}{m_c}\right)^2 \frac{1}{E_g}(2\mu_B H) \quad (C-20)$$

where  $\mu_{\pm}$  is the reduced effective mass for the heavy (-) as light (+) hole transitions to the conduction band:

$$\frac{1}{\mu_{\pm}} = \frac{1}{m_c} + \frac{1}{m_{\pm}} \quad (C-21)$$

Equation (C-20) can be written as

$$\varepsilon(n) = \left(\frac{m}{\mu_-}\right) - [2\alpha \left(\frac{m}{m_c}\right)^2 \frac{1}{E_g}](2n\mu_B H), \quad (n \geq 1) \quad (C-22)$$

Following Vrehan<sup>2</sup> and Reine and coworkers<sup>3</sup> one can measure  $\varepsilon(n)$  directly from the spectra (Figures IV-, 2, 4, 5), for each configuration e.g. H||[100] or H||[110]. One can then plot  $\varepsilon(n)$  vs.  $(2n\mu_B H)$ , and fit a straight line through these points by the method of least squares. The intersection of this line with the  $(2n\mu_B H) = 0$  axis would be just  $(1/\mu_-)$  for that particular orientation e.g. [100] or [110]. This can also show the anisotropy of the heavy hole band. The slope of the line will also determine  $\alpha$ , the nonparabolicity. These measurements

can be used for obtaining preliminary values for some of the parameters to be used for the analysis of spectra as pointed out in Chapter IV.

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  - (i) In Eq.(78)  $-i\gamma$  should be replaced by  $+i\gamma$ , consequently
  - (ii) In Eq.(78) the sign of  $s[6n(n+1)]^{1/2}\gamma$  should be changed, and
  - (iii) In Eq.(81),  $F=-[6n(n+1)]^{1/2}\gamma$ .
  - (iv) In Eq.(83) the following should be added to the right hand side  $-s^4A[B(L_1L_2-L_3^2)-F^2L_2-G^2L_1+2FGL_3]$ .
  - (v) In Eqs.(105 and (106),  $(n-\frac{3}{2})$  should be replaced by  $(n+\frac{1}{2})$ ,
  - (vi) In Eq.(108) in the second line  $\frac{A+B}{E_g+\Delta}$  should be replaced by  $\frac{AB}{E_g+\Delta}$ .
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